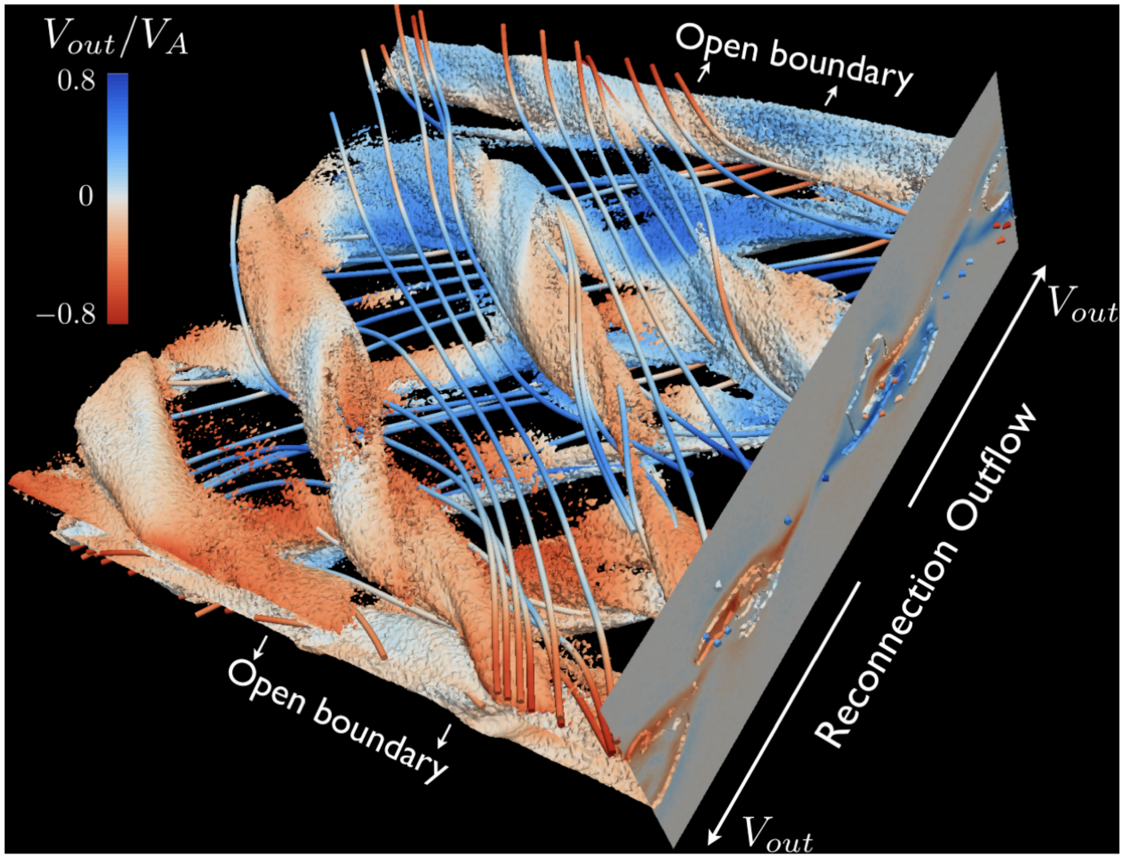
Advances in Kinetic Plasma Simulation with VPIC and Roadrunner



Kevin Bowers*, Brian Albright, Lin Yin, Bill Daughton, Vadim Roytershteyn, Ben Bergen and Tom Kwan
Los Alamos National Lab
* Guest Scientist

Overview

The Software

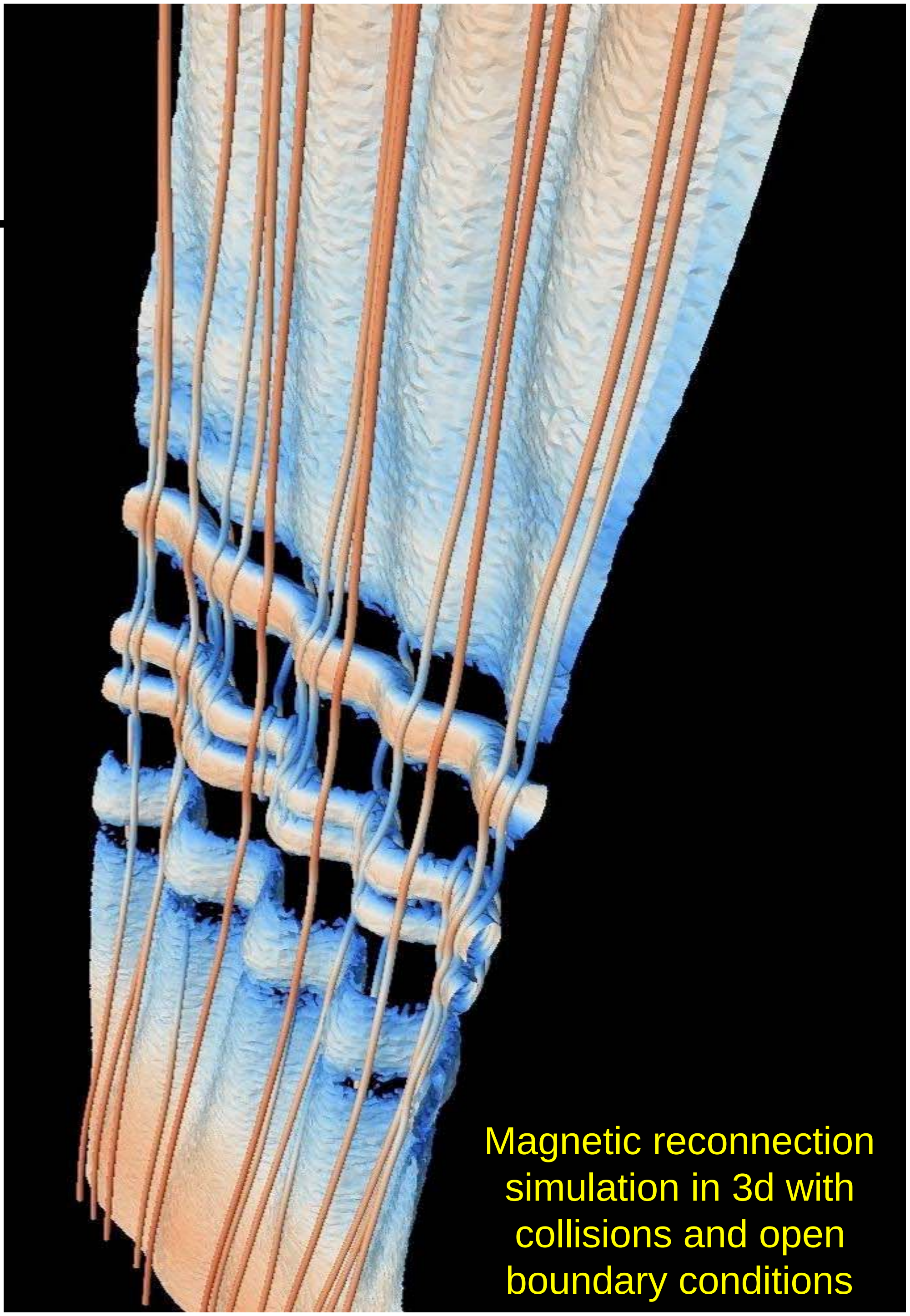
- VPIC: A 3d electromagnetic relativistic particle-in-cell simulation code

The Supercomputer

- Roadrunner: A petascale heterogeneous Cell / Opteron cluster

The Science

- Laser-Plasma Interaction in Inertial Confinement Fusion
- Laser Ion Acceleration
- Magnetic Reconnection


Magnetic reconnection simulation in 3d with collisions and open boundary conditions

Choir Preaching

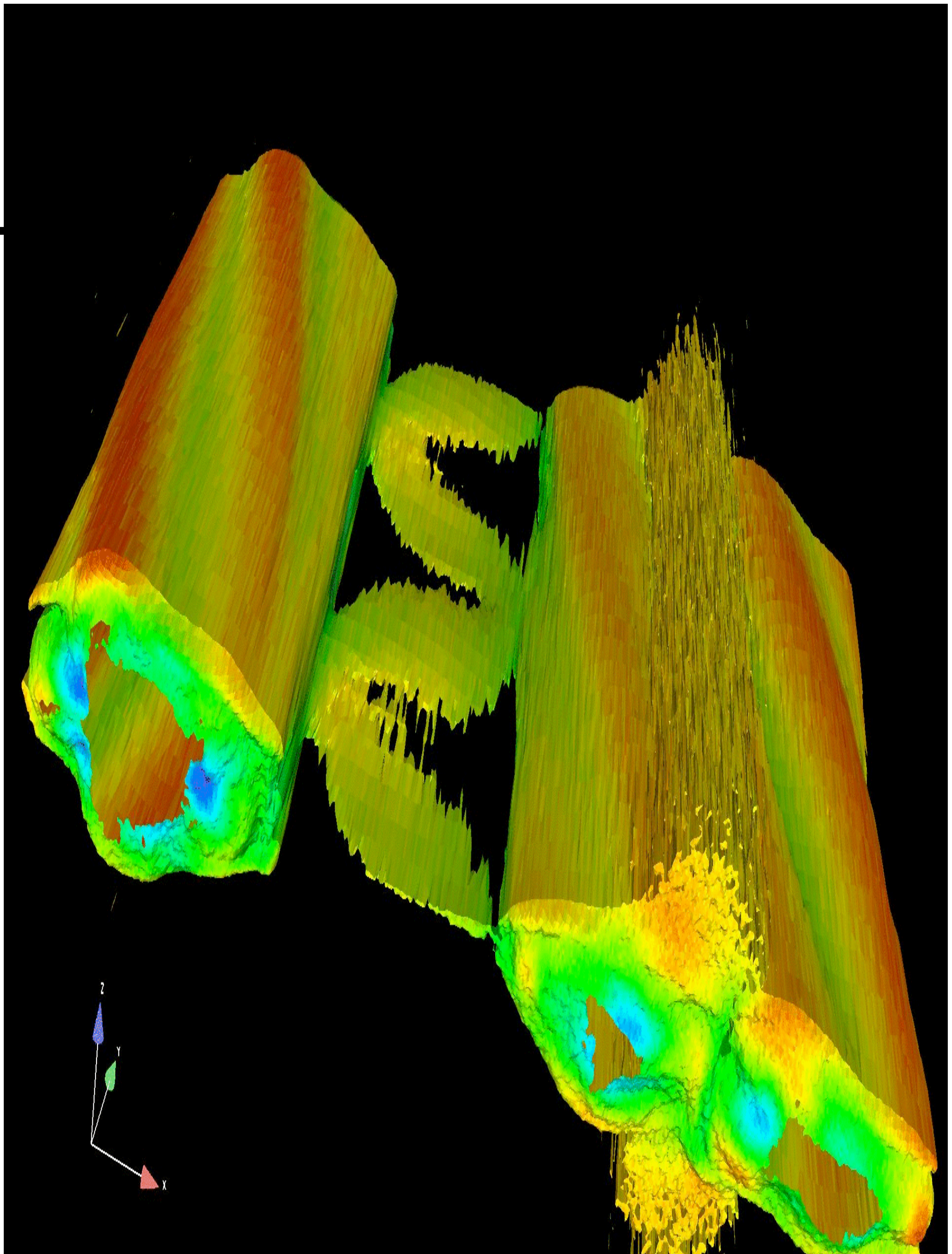
Petaflops today

Exaflops in 10 years

Few experimental and observational capabilities will see a comparable increase

Computational science well positioned for discoveries in biology, chemistry, climate, cosmology, energy, materials, plasmas ...

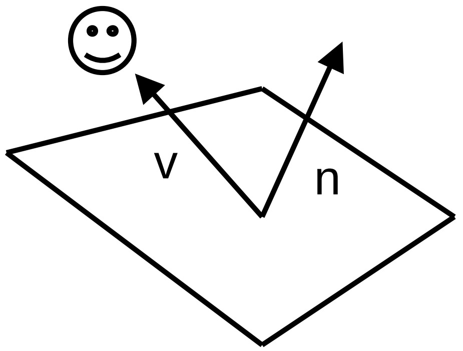
Los Alamos



3d Collisionless Pair-Plasma Magnetic Reconnection (Yin *et al*, Phys Rev Lett, 2008)

Modern CPUs Optimized for Games

$$\begin{bmatrix} x' \\ y' \\ z' \\ 1 \end{bmatrix} = \begin{bmatrix} r_{xx} & r_{xy} & r_{xz} & t_x \\ r_{yx} & r_{yy} & r_{yz} & t_y \\ r_{zx} & r_{zy} & r_{zz} & t_z \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}$$



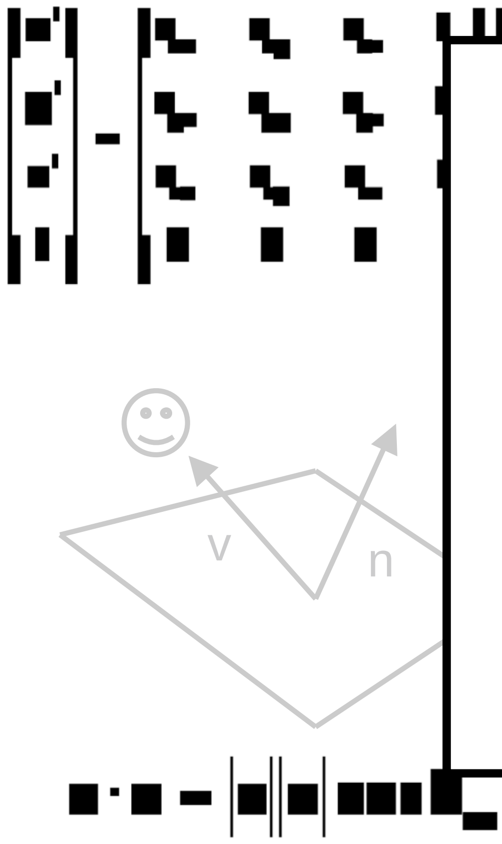
$$v \cdot n = |v||n| \cos\theta_{vn}$$

Floating point intensive games use small matrix / short vector ops in single precision

Single precision 4-vector SIMD (<u>S</u>ingle-<u>I</u>nstruction-<u>M</u>ultiple-<u>D</u>ata) extensions common

Not optimized for traditional double precision large vector operations

Modern CPUs Optimized for Games



Floating point intensive games use
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Multiple-Data)

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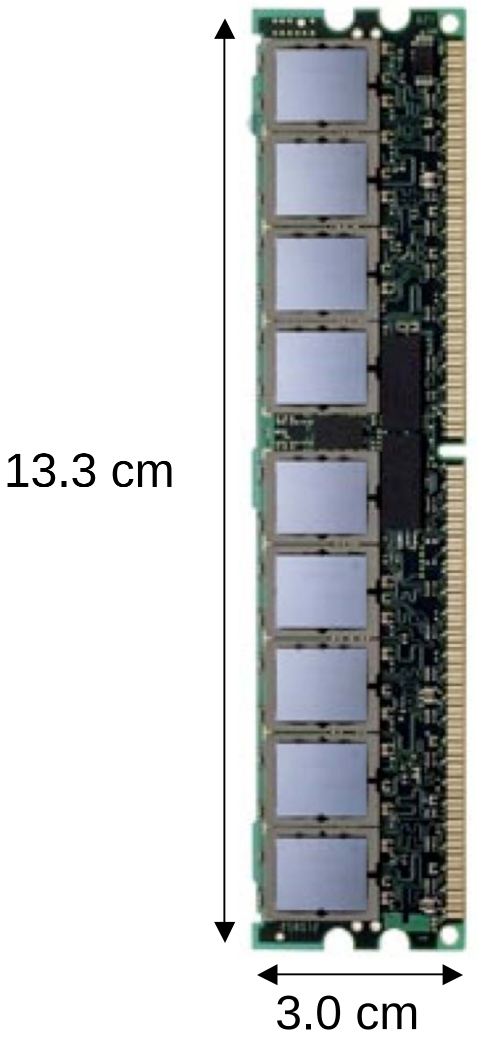
operations

Roadrunner based on a chip originally designed for the Sony Playstation 3 videogame console

The Speed of Light is Too Slow



Consider a registered ECC DDR2-DIMM in a node with 3.2 GHz dual-issue 4-vector SIMD cores (e.g., Roadrunner)

Characteristic time for a signal at the effective speed of light to travel around the DIMM is ~3.2 ns

This alone is ~10 clocks

Time enough for ~80 flops / core

This is optimistic; many other delays

The Speed of Light is Too Slow

Consider a registered ECC DDR2-

Hz dual-

(e.g.,

nal at the

avel

s

s / core

Due to physical limitations, moving data between, and even within, modern microchips is more time consuming than performing computations

This is optimistic; many other delays

Overview

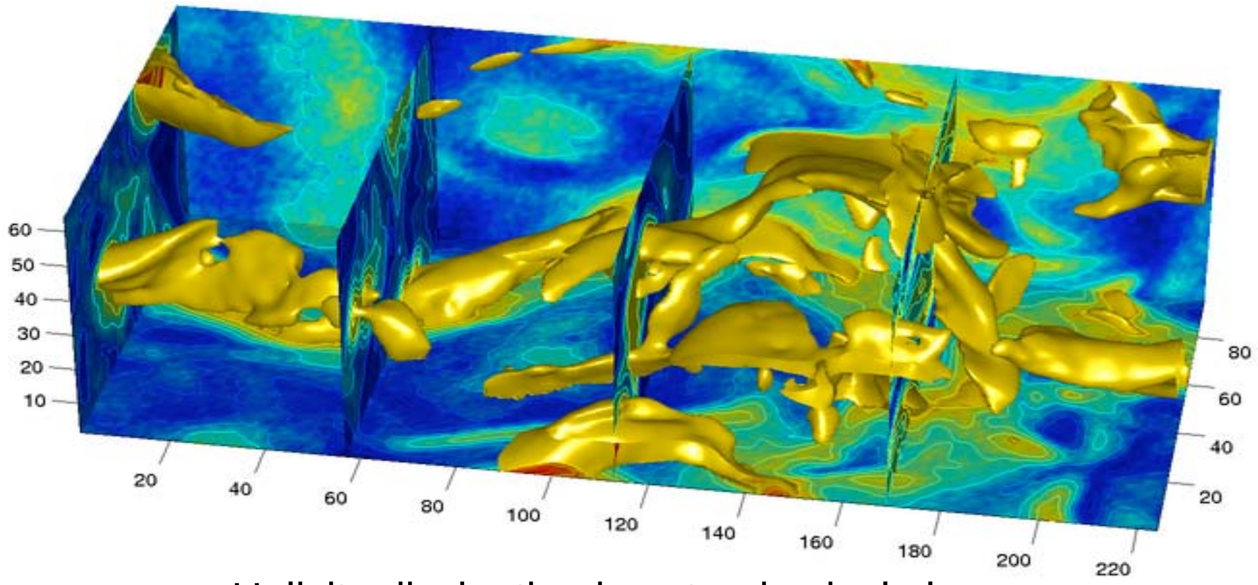
The Software

- VPIC: A 3d electromagnetic relativistic particle-in-cell simulation code

Modeling capabilities

Comparison with other techniques

Implementation considerations



Helicity dissipation in astrophysical plasma
(Bowers and Li, Phys Rev Lett, 2006)

What does VPIC do?

VPIC integrates the relativistic Maxwell-Boltzmann system in a linear background medium for multiple particle species,

$$\partial_t f_s + c\gamma^{-1}\vec{u}\cdot\nabla f_s + \tfrac{q_s}{m_s c}\left(\vec{E} + c\gamma^{-1}\vec{u}\times\vec{B}\right)\cdot\nabla_u f_s = \left(\partial_t f_s\right)_{coll}$$

$$\partial_t \vec{E} = \varepsilon^{-1}\nabla\times\mu^{-1}\vec{B} - \varepsilon^{-1}\vec{J} - \varepsilon^{-1}\sigma\vec{E}$$

$$\partial_t \vec{B} = -\nabla\times\vec{E},$$

in time with an explicit-implicit mixture of velocity Verlet, leapfrog, Boris rotation and exponential differencing based on a reversible phase-space-volume conserving 2nd order Trotter factorization.

Direct discretization of f_s is prohibitive; f_s is sampled by particles,

$$d_t\vec{r}_{s,n} = c\gamma_{s,n}^{-1}\vec{u}_{s,n} \qquad d_t\vec{u}_{s,n} = \tfrac{q_s}{m_s c}\left(\vec{E}\Big|_{\vec{r}_{s,n}} + c\gamma_{s,n}^{-1}\vec{u}_{s,n}\times\vec{B}\Big|_{\vec{r}_{s,n}}\right).$$

Particles obey the same Boltzmann equation outside of collisions.

A smooth J is extrapolated from the particles; as a result, E, B and J can be sampled on a mesh and interpolated to and from particles.

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[illegible]

in time with an explicit-[illegible] let, leapfrog, Boris rotation and exponentia[illegible] ersible phase-space-volume conserving 2nd [illegible]

Theoretical explanation mostly useful for making babies cry

Direct discretization of [illegible] by particles,

[illegible]

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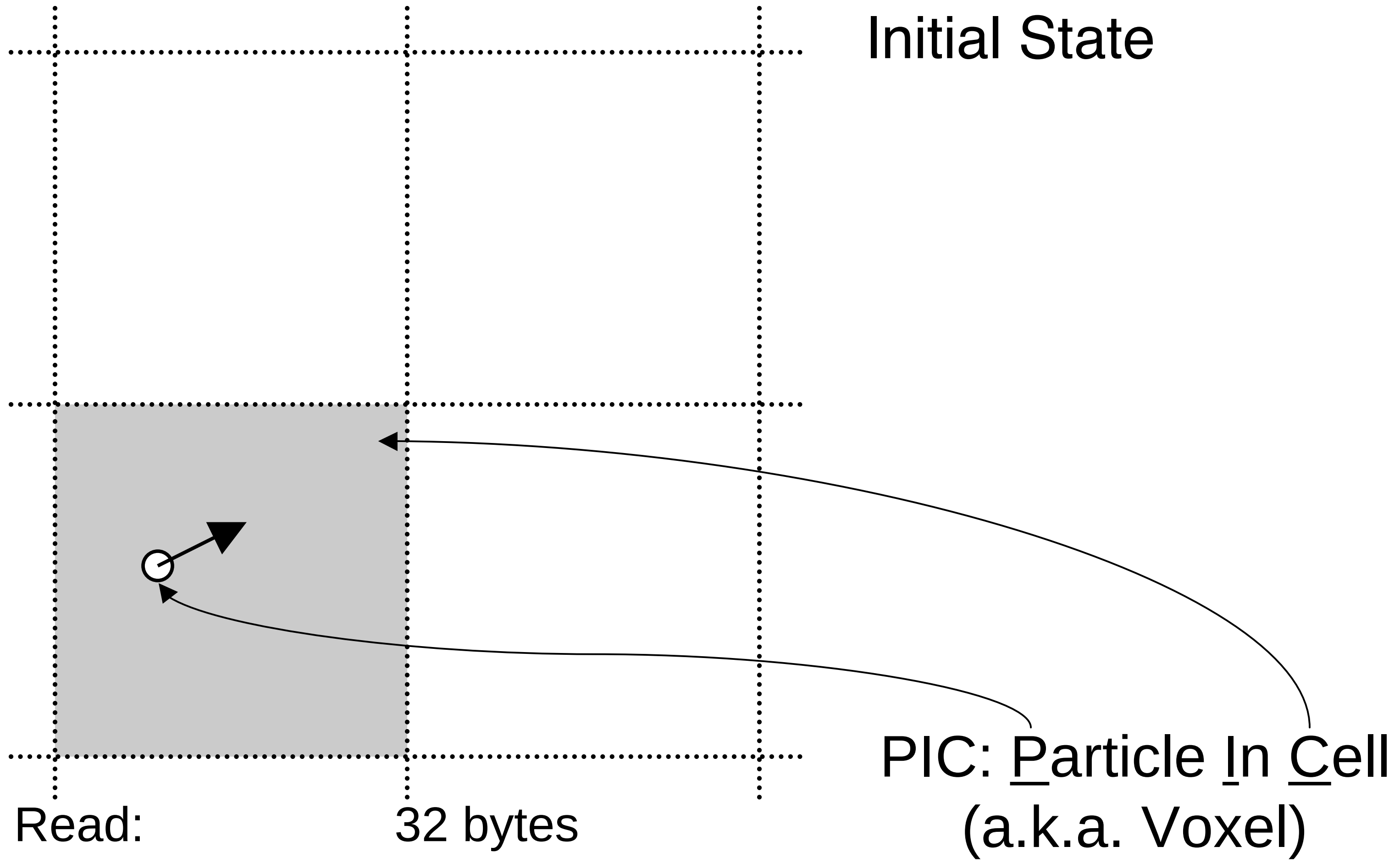
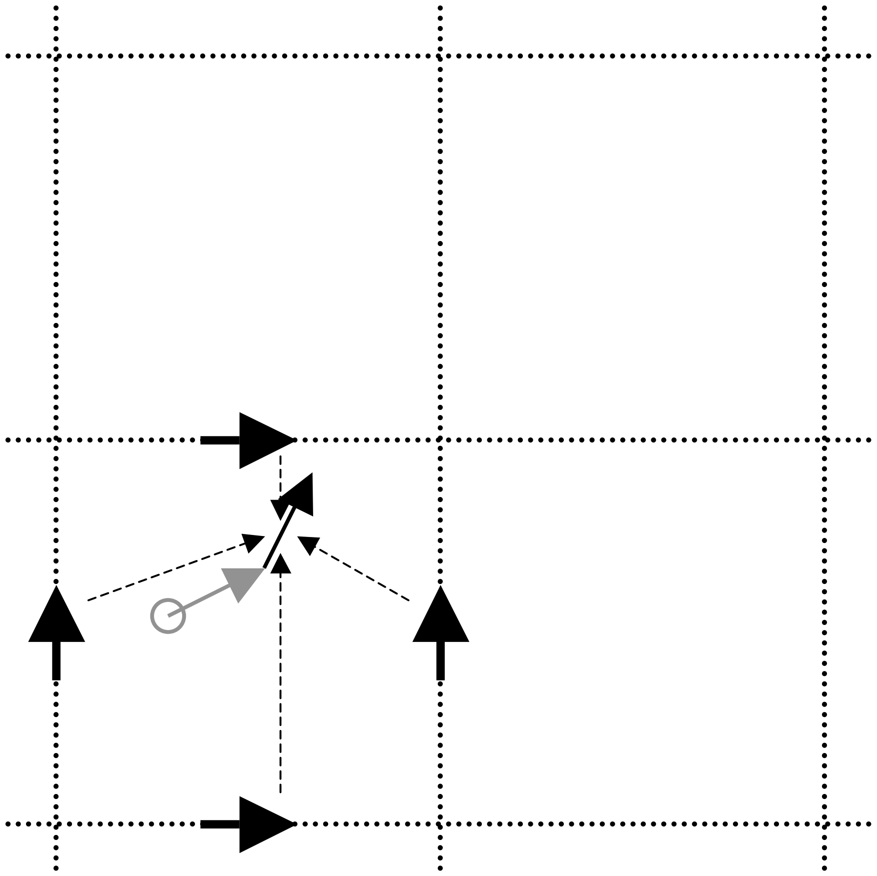
What does VPIC really do?



Read:	32 bytes
Write:	0 bytes
Compute:	0 flop

What does VPIC really do?



Initial State

Interpolate *E* and *B*

Read:	72 bytes
Write:	0 bytes
Compute:	27 flop

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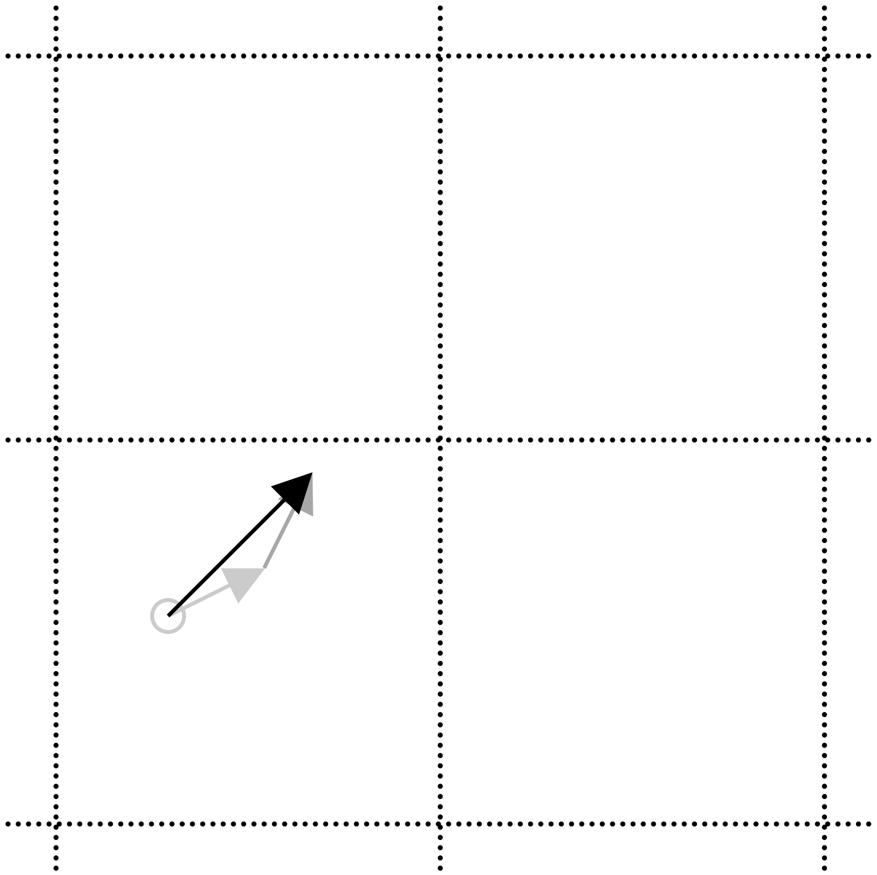

Initial State

Interpolate *E* and *B*

Update *u*

Read:	0 bytes
Write:	0 bytes
Compute:	107 flop

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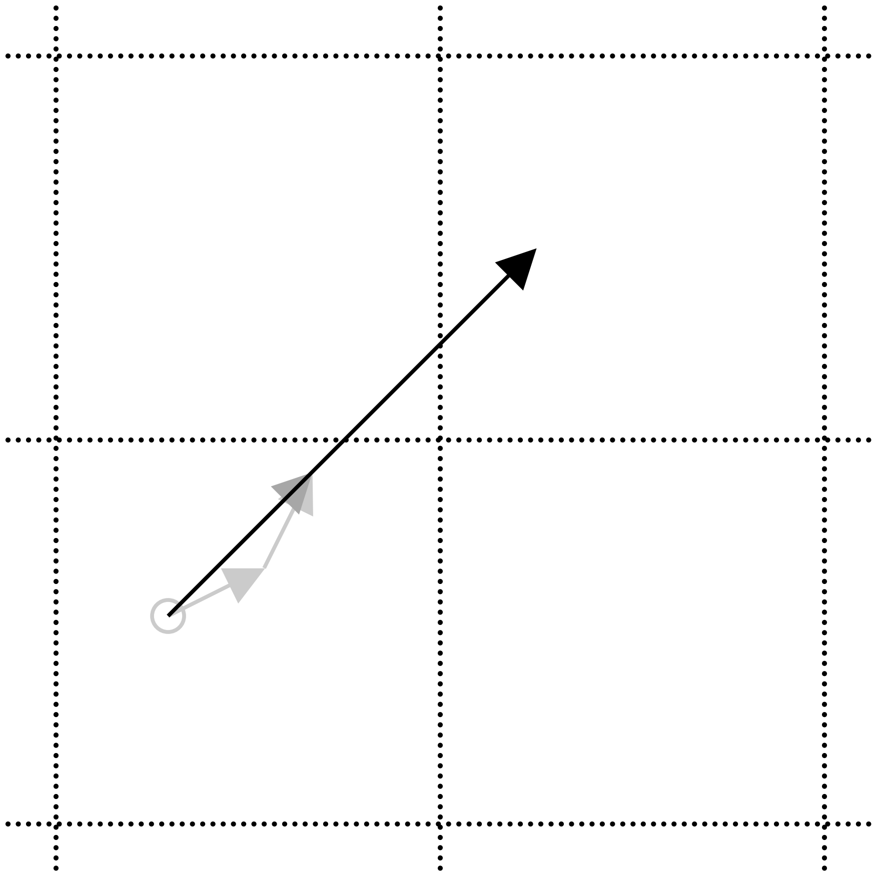


Initial State

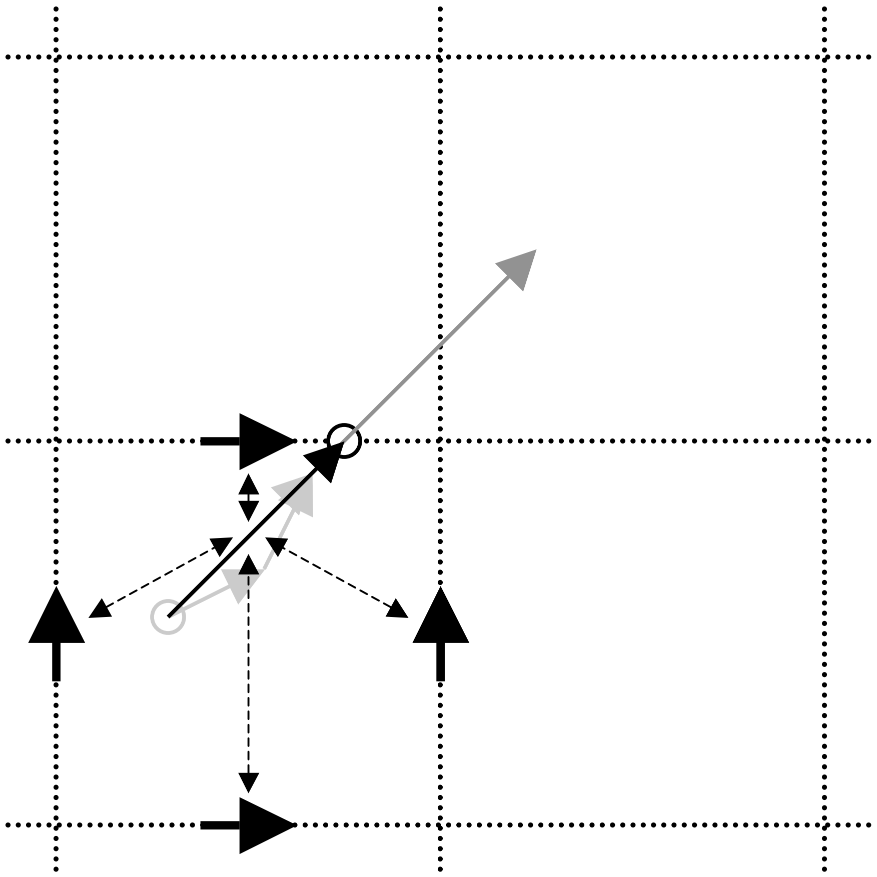
Interpolate *E* and *B*

Update *u*

Compute Motion

Read:	0+48 bytes
Write:	0+48 bytes
Compute:	42+70 flop

What does VPIC really do?



Initial State

Interpolate *E* and *B*

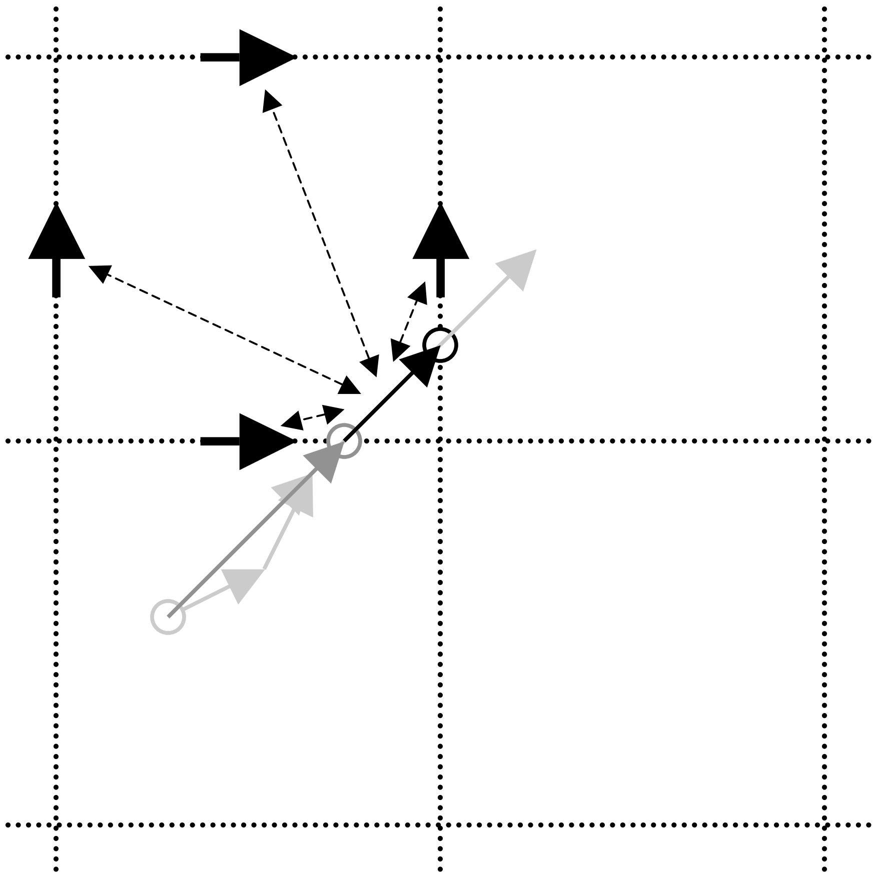
Update *u*

Compute Motion

Update *r* and *J*

Read:	56 bytes
Write:	48 bytes
Compute:	168 flop

What does VPIC really do?



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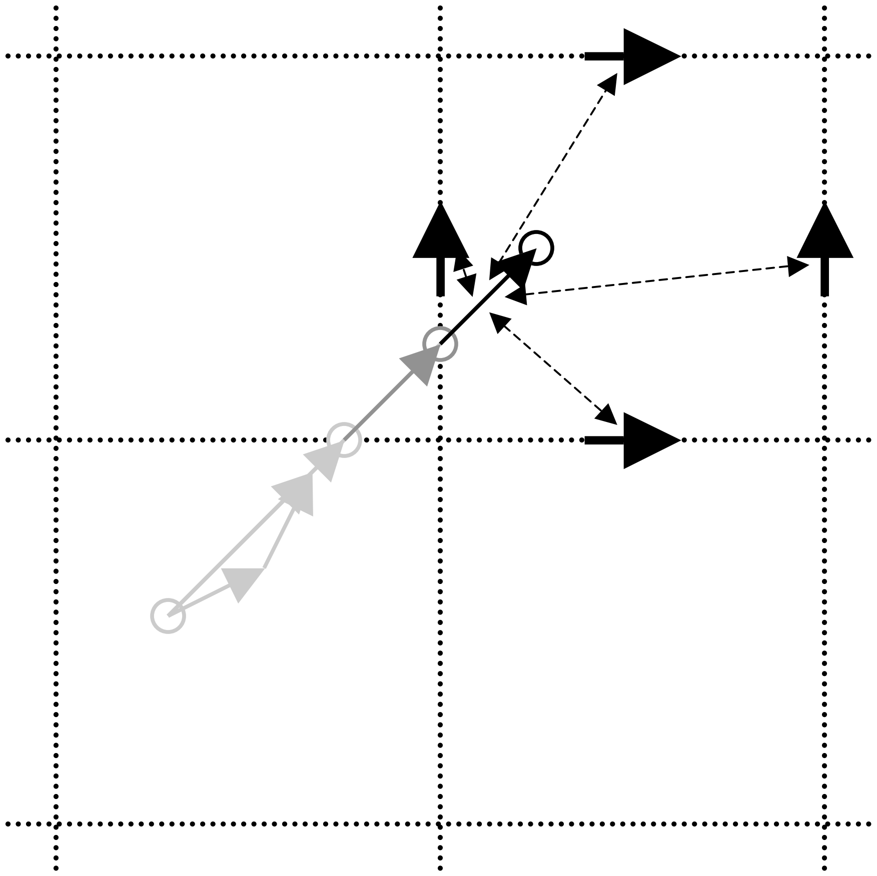

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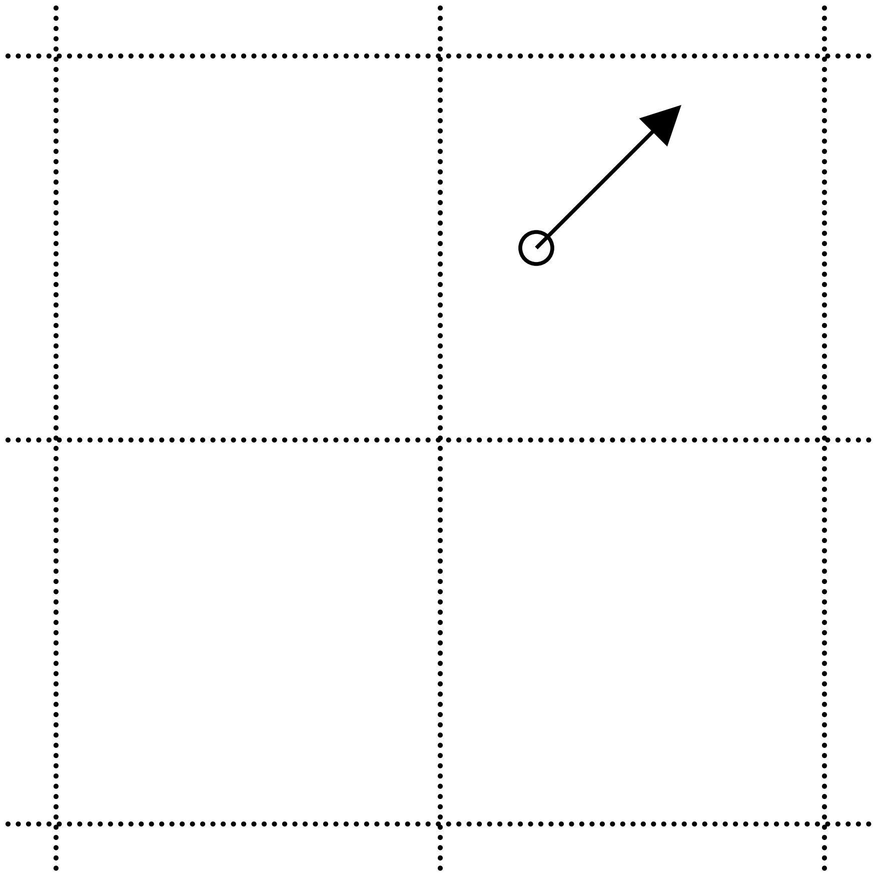

Initial State

Interpolate *E* and *B*

Update *u*

Compute Motion

Update *r* and *J*

Update *r* and *J*

Update *r* and *J*

Final State

Read:	0 bytes	**Net Read:**	152+ 56 n_c bytes
Write:	32 bytes	**Net Write:**	80+ 48 n_c bytes
Compute:	0 flop	**Net Compute:**	246+168 n_c flop

Why use PIC?

Vlasov codes model similar equations

- But do not scale to high dimensional systems

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Molecular dynamics closely related

- But orders of magnitude more expensive ...

MD versus PIC

MD focus is short range

- Necessary when nearby interaction potential energy >> thermal energy
- Difficult for particles to represent many atoms
- ***Flops / particle / step large (10^3 - 10^4)***

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PIC focus is long range

- Useful when nearby interaction potential energy << thermal energy
- Approximates short range interactions
- ***Flops / particle / step small (~10^2)***

Typical VPIC Simulations

Many particles / node (10^7 - 10^8)

- Particle data does not fit in cache
- >90% expense is particle pushing

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Many voxels / node (10^4 - 10^5)

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- Many particles / voxel (10^2 - 10^4)

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- Speed of light well resolved and $v<c$

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Internode communications naturally optimal

- Communication every step, but, because of finite *c*, data needed on a node already there or nearby

Typical VPIC Simulations

Many particles / node (10^7 – 10^8)

- Partic
- >90%

Many vo

- Field
- Many

Few vox

- Spee

Internod

- Com ite *c*, data needed on a node already there or nearby

VPIC isn't like a matrix calculation with O(N^3) compute on O(N^2) data

Low compute to data motion ratio (~1 flop / byte) makes high performance hard to achieve

Performance limited by local data motion

Bad Ideas

Absolute particle coordinates	***Destroys precision*** Bits wasted resolving voxel indices ***Slow interpolation*** Float - int casts (or worse)

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Field samples used for interpolation	***Too few "ways" to keep track*** 29 diff memory regions accessed / particle

Bad Ideas

Absolute particle coordina | *Destroys precision* s

Unsorted particles

Advance several p

Each co stored in

Field sa for interpolation | 29 dim memory regions accessed / particle

If VPIC were implemented conventionally, ~31 physical DRAM transfers / particle / step and not many flops to show for them

Need data flow optimization techniques

Good Ideas

Voxel index + offset particle coordinates	***Maximizes precision*** Bits conserved; critical in single precision
	Fast interpolation No casts; almost trivial computation
Sorted particles	***Cache hits*** Field data approximately streamed
Advance done in a single pass	***Bandwidth conserved*** Particle data touched once / step
Similar components grouped together	***Bandwidth conserved*** Large aligned accesses
Precompute voxel interpolation coeffs	***Many "ways" to keep track*** 2 diff memory regions accessed / particle

No Apologies

VPIC designed with single precision in mind

- Half bytes moved and wider SIMD available

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Usually, discretization error >> single precision error

- Single precision okay if very carefully implemented
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- Extensive convergence studies and validation against theory, experiment, double precision codes

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Stabilized to the point where each voxel has identical numerical properties regardless how the voxel mesh is translated, oriented or reflected

No Apologies

VPIC designed with single precision in mind

- Half b

Usually rror

- Singl nted
- Doub lically
- Exter
  agair codes

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identi ow the
vox cted

When in single precision, developers care <u>more</u> about arithmetic error

Unlike double precision, ignoring it often leads to catastrophes

We die a little bit on the inside when CPUs and compilers take short cuts (they often do)

Overview

The Supercomputer

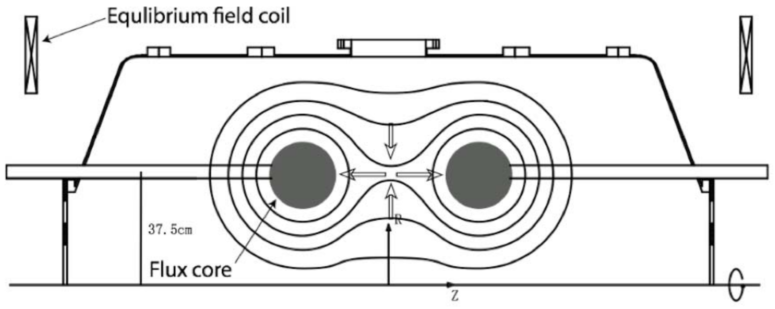
- Roadrunner: A petascale heterogeneous Cell / Opteron cluster

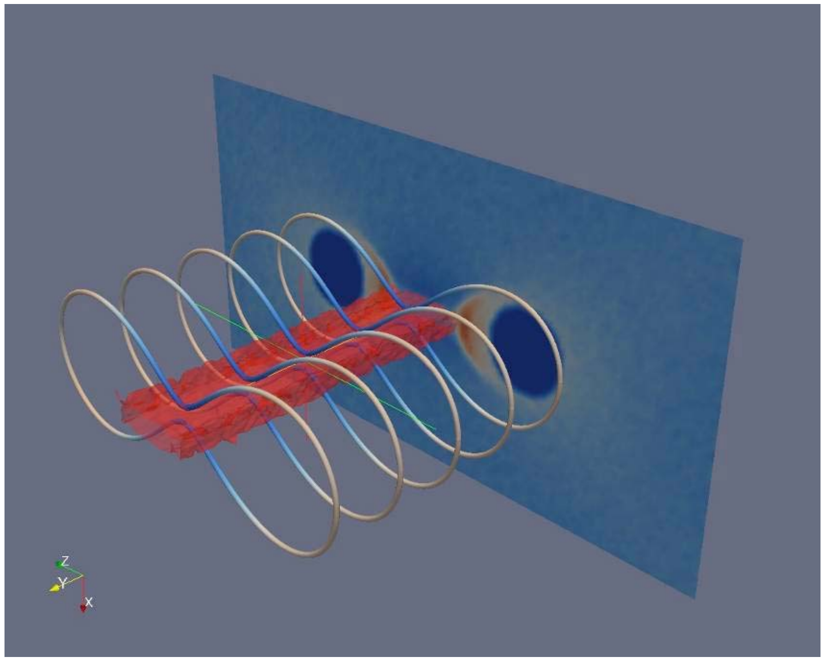
Hardware Description

Porting Details

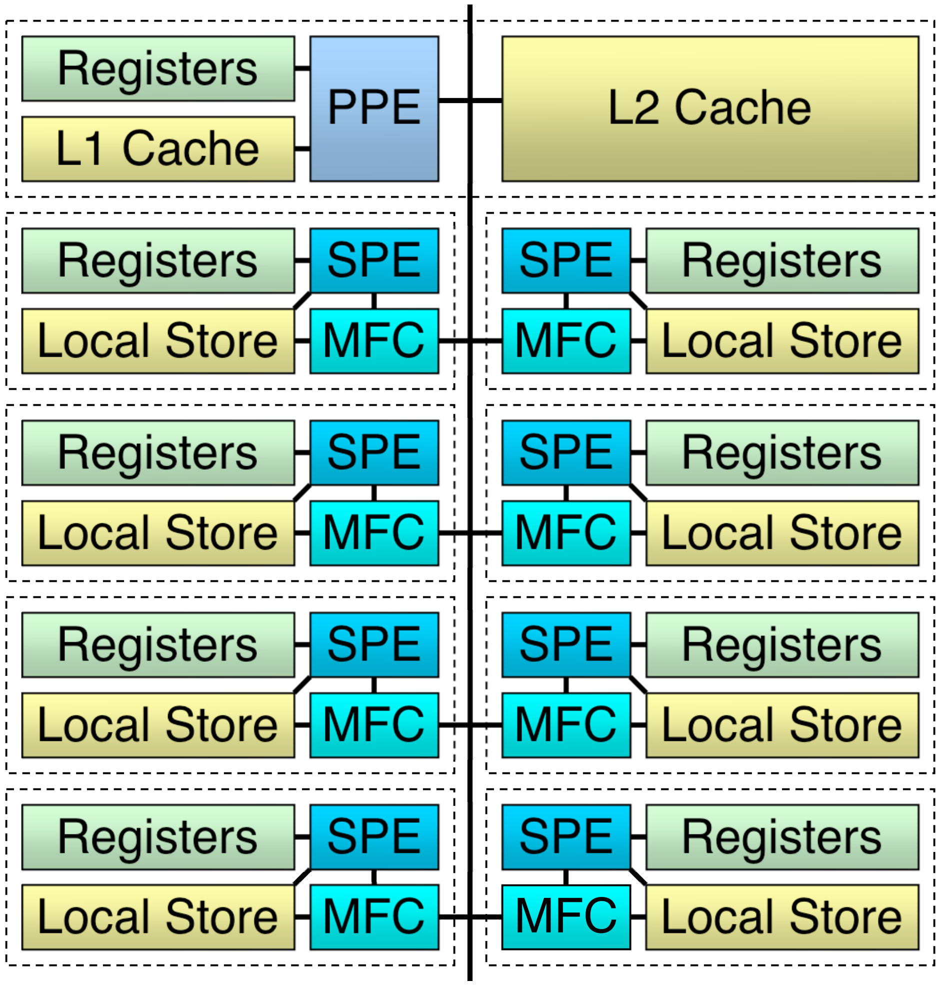
Measured performance

Preliminary 3d Collisional VPIC Simulation of MRX (Magnetic Reconnection eXperiment)





Cell Broadband Engine



1 general purpose core, "PPE"

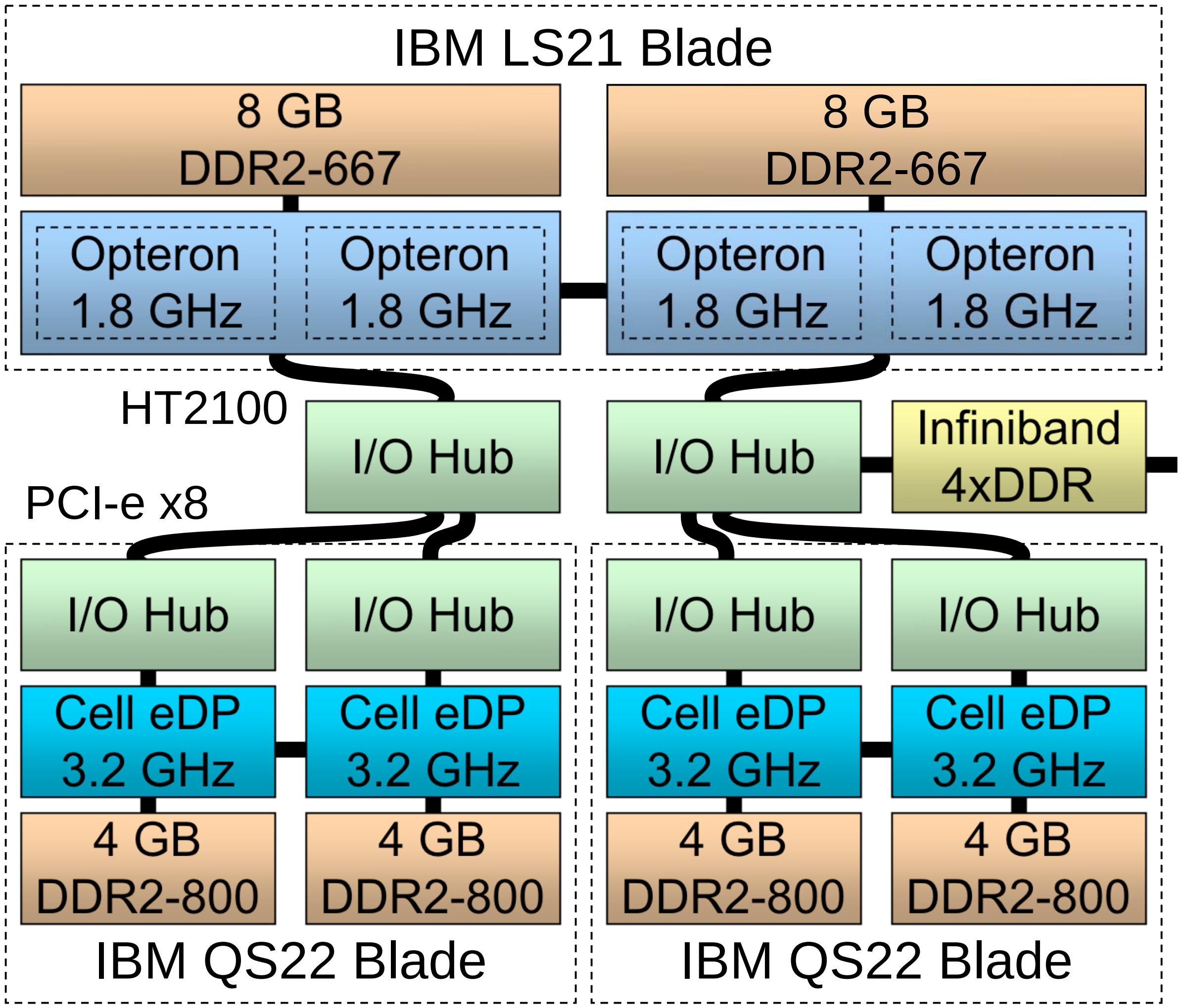
8 special 4-vector SIMD cores, "SPE"

Each SPE can only directly access its 256KB "local store"

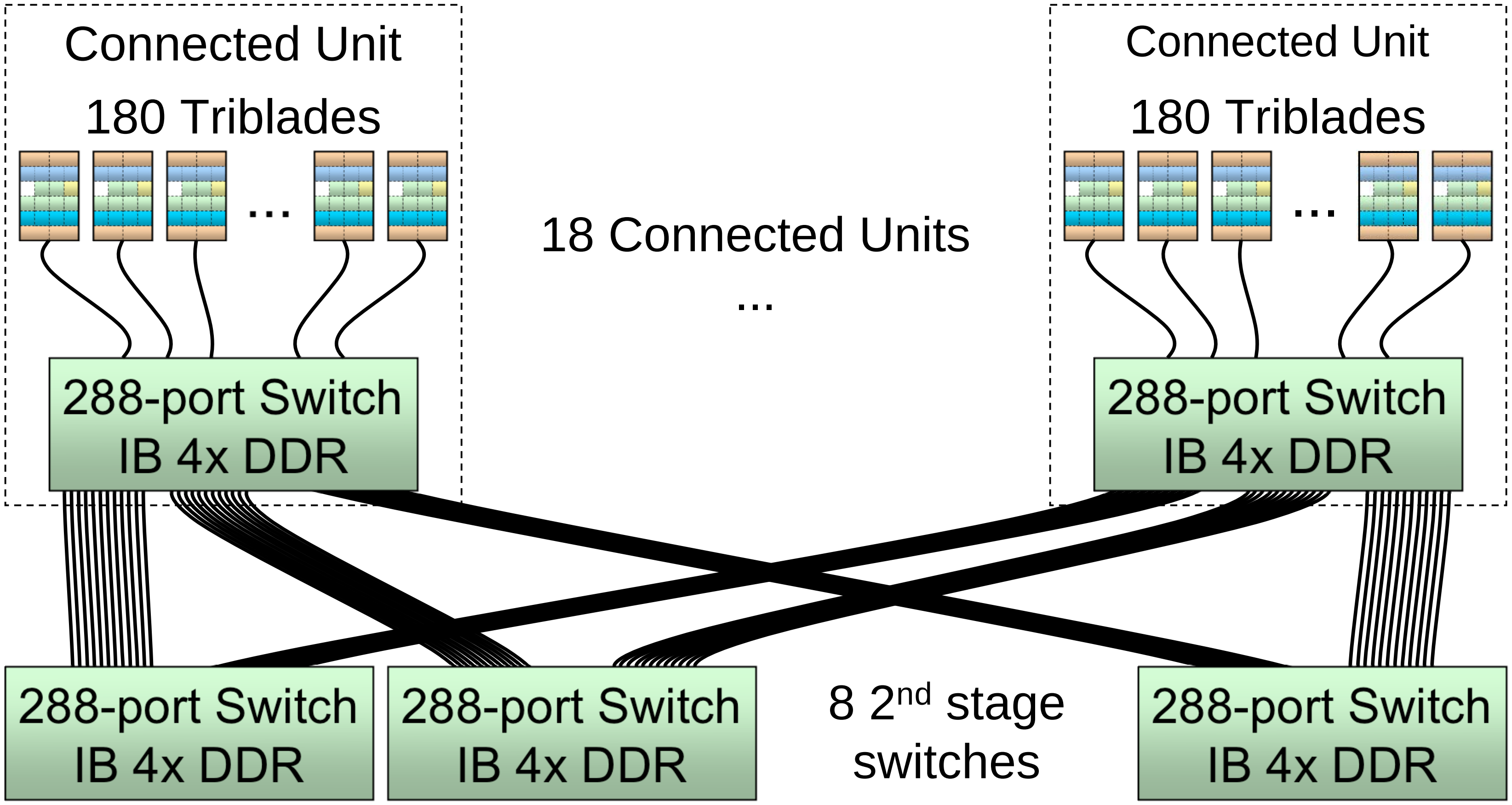
Local store like cache but memory transfers explicitly managed by "MFC"

Triblade Compute Nodes

Opteron cores one-to-one with Cell eDPs (2 GB/s bandwidth)



Roadrunner



12,960 Opteron cores - ***0.1 Pflop/s (s.p.)***

12,960 Cell eDP chips - ***3.0 Pflop/s (s.p.)***

Porting

Observations

- Most compute in the SPEs
- SPE / Cell DRAM bandwidth (25 GB/s) >>
  SPE / Opteron DRAM bandwidth (2 GB/s)
- Bandwidth off-node same for Cell and Opteron (IB)

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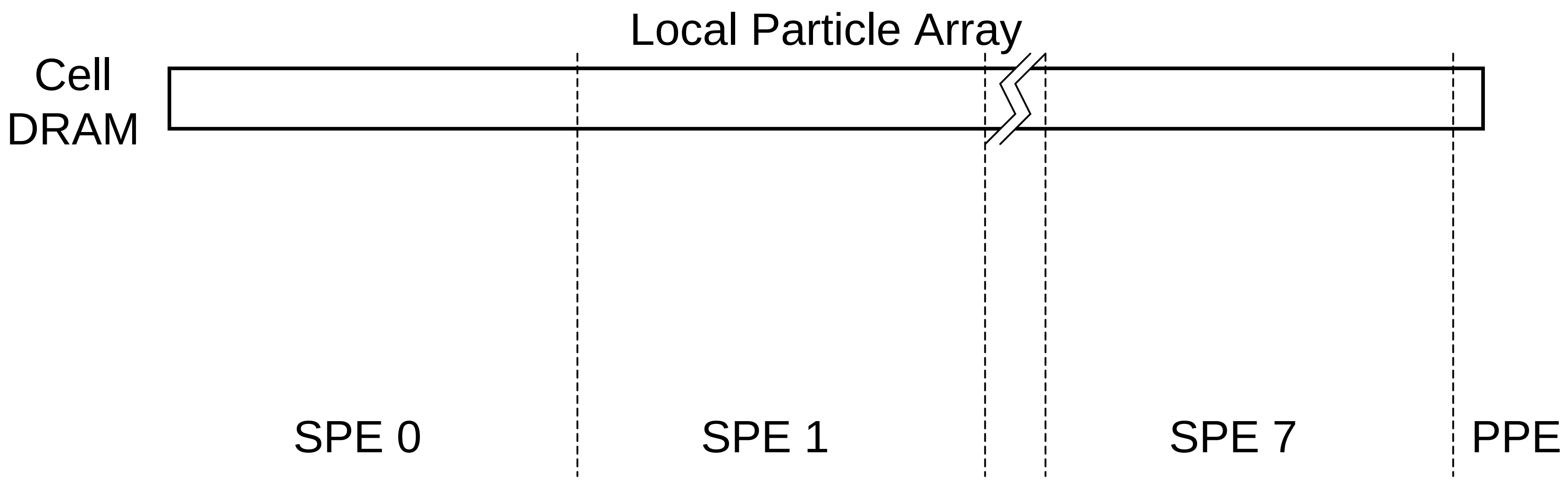
Strategy: **Flatten Roadrunner**

- All calculations done on Cells
- All data stored in Cell DRAM
- Opterons relay Cell communication and I/O

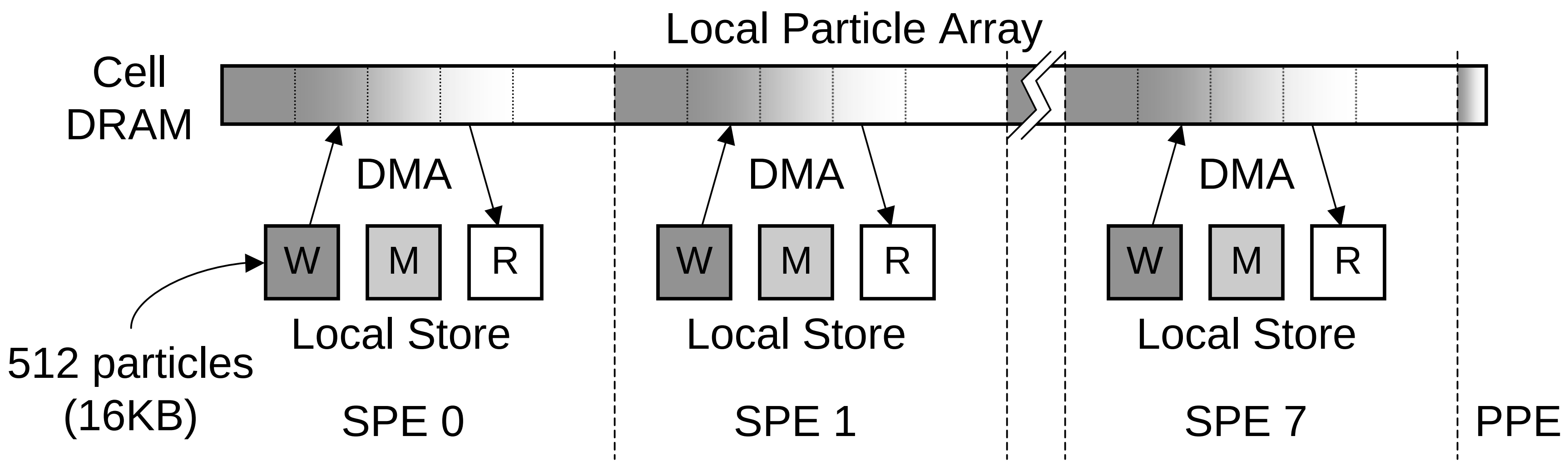
SPE Accelerated Particle Advance



Each SPE assigned a segment containing a multiple of 16 particles and an exclusive current accumulator

The PPE assigned leftover particles

SPE Accelerated Particle Advance



Each SPE assigned a segment containing a multiple of 16 particles and an exclusive current accumulator

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SPEs stream through segments with triple buffering in blocks of 512 particles

SPE Accelerated Particle Advance

The heart of it all: A 512-line part read-only / part write-back software cache handles random access

- **Fully-associative:** A line can hold any voxel's data
- **Least-recently-used:** New data evicts oldest data

The last 512 unique requests guaranteed in cache

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The last 512 unique requests <u>guaranteed</u> in cache

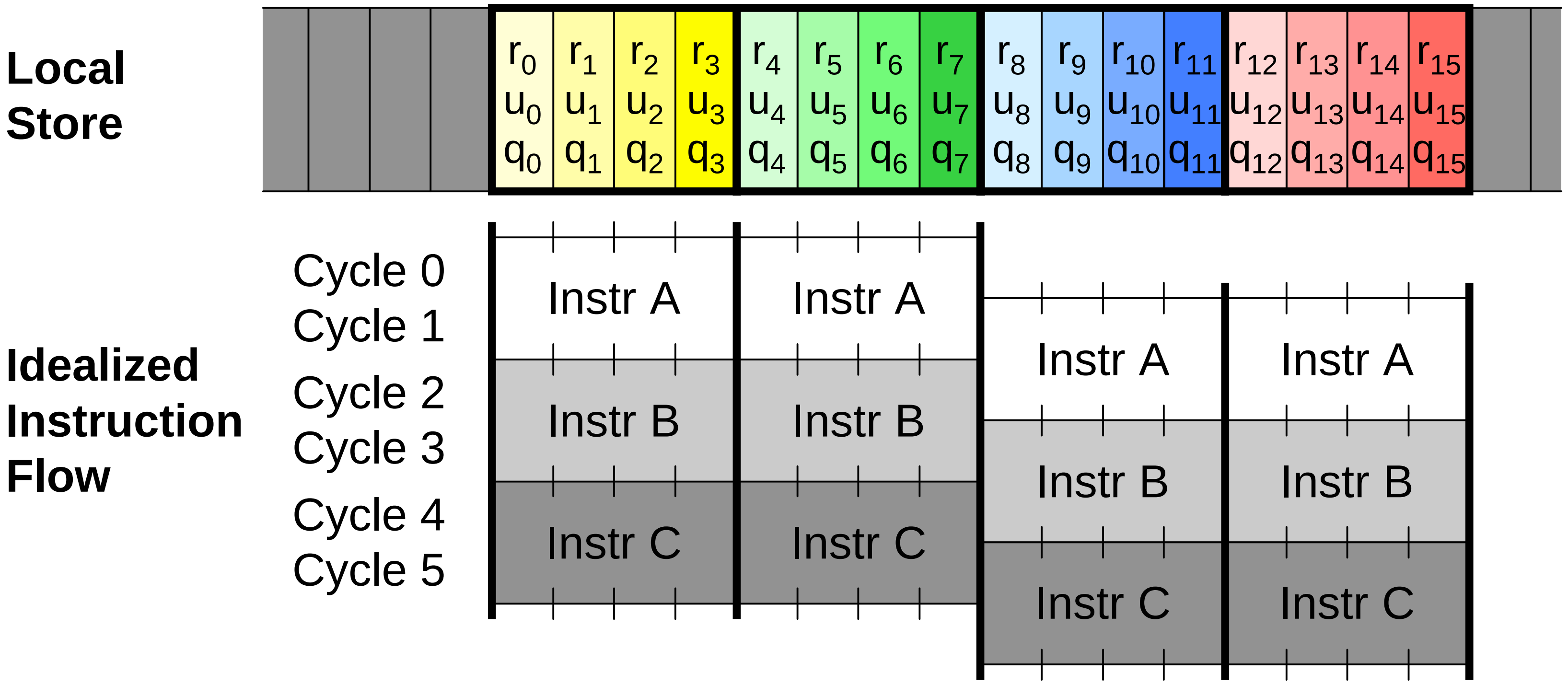
`cache_fetch` called on all 512 particles in a new block

- Most are hits; DMA transfers started for misses
- Returns which lines will hold the voxels' data

`cache_wait` then completes any pending fetches

`cache_fetch` non-trivial internally but a fast *O*(1)

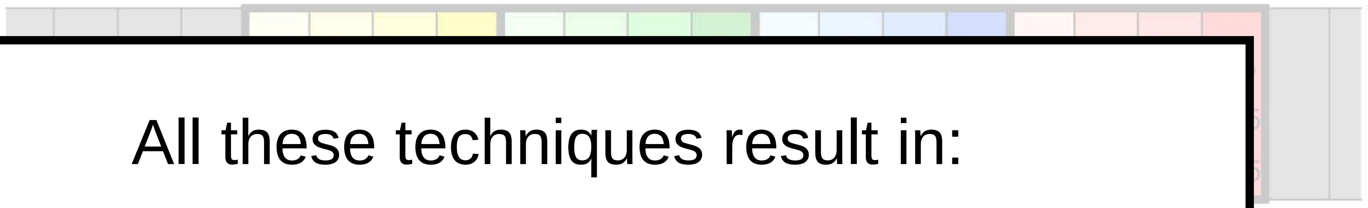
SPE Accelerated Particle Advance



Particles processed 16 at a time

- Original x86 4-vector SIMD kernel hand unrolled and modulo scheduled by 4; register file size (128), pipeline hazards and local store limit further unrolling

SPE Accelerated Particle Advance



All these techniques result in:

A SPE kernel that operates exclusively out of local store

Most SPE registers used
Most local store used
All 32 DMA channels / SPE used
Most DMA transfers overlapped
Many independent SIMD instructions
Minimal DMA transfers / particle

Kernel Performance

162.0 million cold particles advanced / s / Cell

÷ 10.3 million cold particles advanced / s / Opteron

15.7x speedup

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÷ **8.0x** more SPE cores than Opteron cores

1.1x clock-for-clock speedup, in spite of SPE minimalism and VPIC's tuning for x86

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0.517 *Pflop/s on all* 18 *Roadrunner Connected Units*

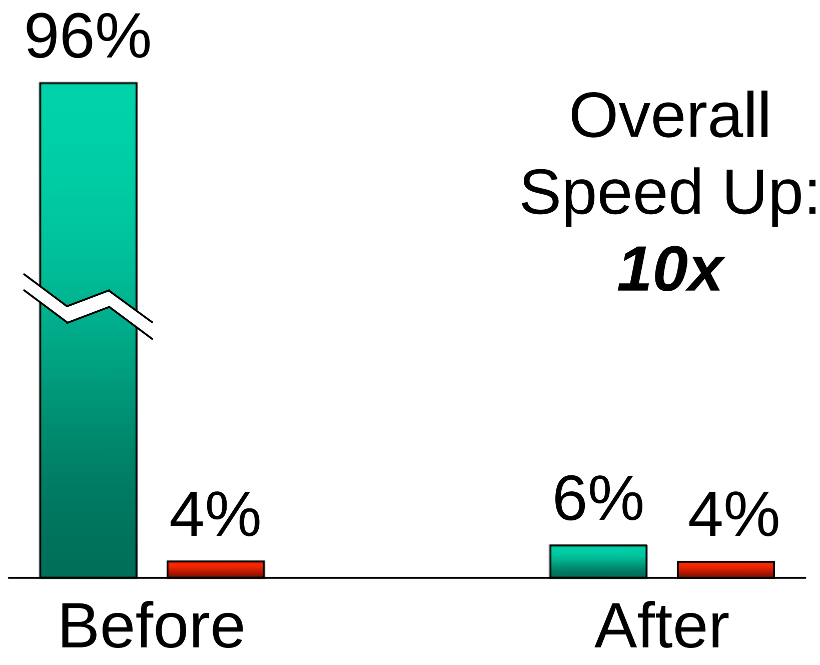
Need 203,000 Opteron cores for similar performance

Amdahl's Whack-a-Mole

Particle advance accelerated 15.7x

Amdahl's Law:

Rest of code relatively more costly



Overall
Speed Up:
10x

Amdahl’s Whack-a-Mole

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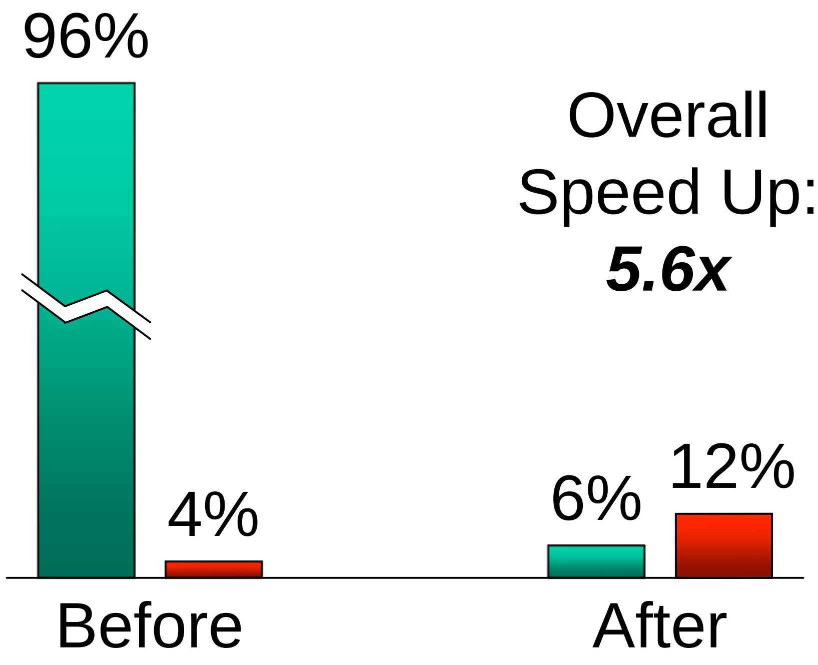
Amdahl’s Street Justice:

Rest of code <u>absolutely</u> more costly

PPE cores less powerful than Opteron cores



Overall
Speed Up:
5.6x

Amdahl's Whack-a-Mole

Particle advance accelerated 15.7x

Amdahl's Street Justice:

Rest of code <u>absolutely</u> more costly

PPE cores less powerful than Opteron cores

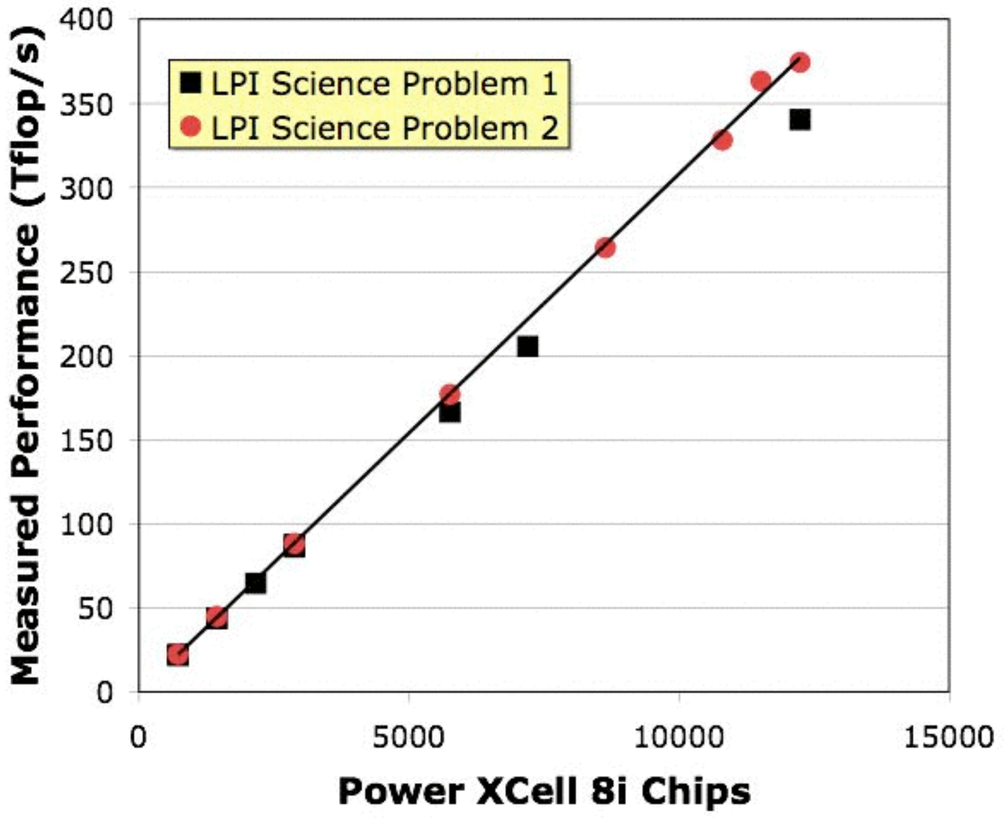
End-to-end performance more sensitive to unaccelerated kernels than conventional platforms. Particle sort and many field update kernels were also SPE accelerated (several fold speedups).

Amdahl bottlenecks are now frequently one-off user-provided application-specific in-situ diagnostics. User experience, improved development models needed.

End-to-End Performance

Two simulations in LPI parameter study (Albright *et al*, Phys Plasmas, 2008) used to benchmark weak scaling

Same physics but 10x faster



Trillion-particle simulations at* 0.374 *Pflop/s sustained on* 17 *CUs (Bowers* et al, *SC08)

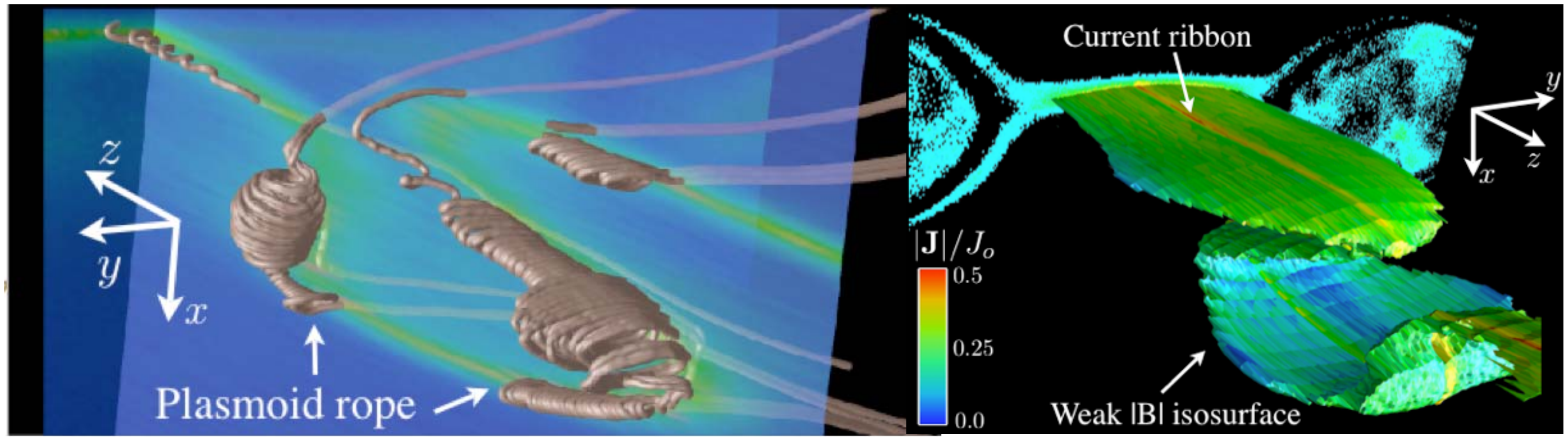
Overview

The Science

- Laser-Plasma Interaction in Inertial Confinement Fusion
- Laser Ion Acceleration
- Magnetic Reconnection

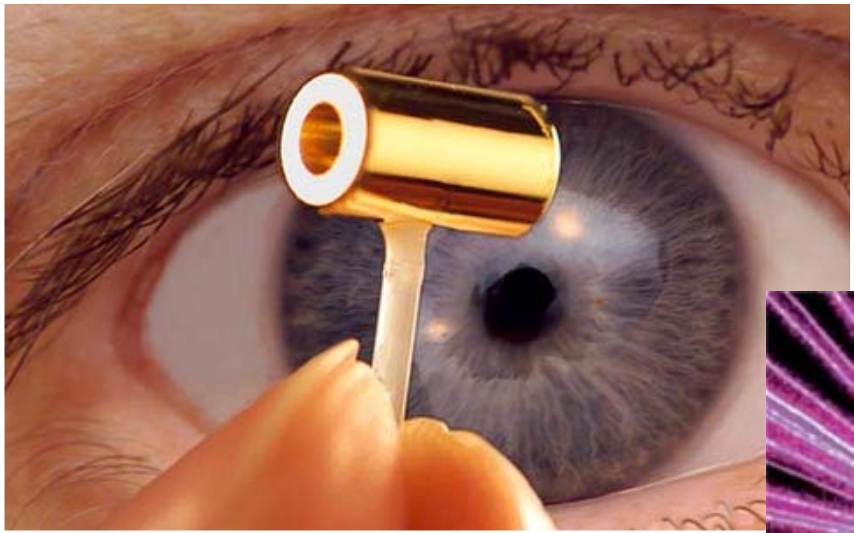
For each, a brief overview of current research with VPIC on Roadrunner

Conclusions

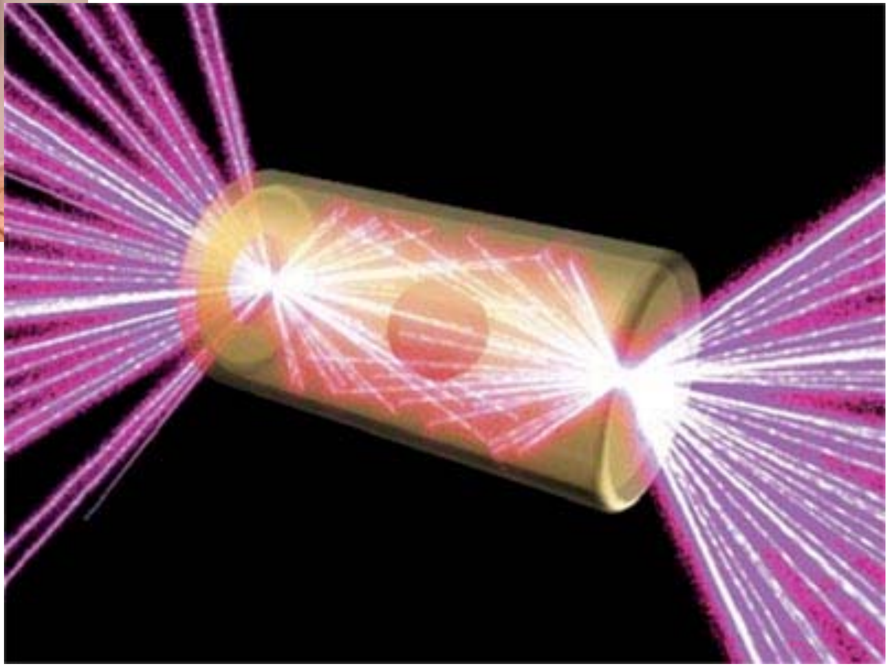


Magnetic Island Detachment (Yin *et al*, Phys Rev Lett, 2008)

Inertial Confinement Fusion



Lasers implode a fusion fuel capsule to "ignite" it; thermonuclear burning plasma

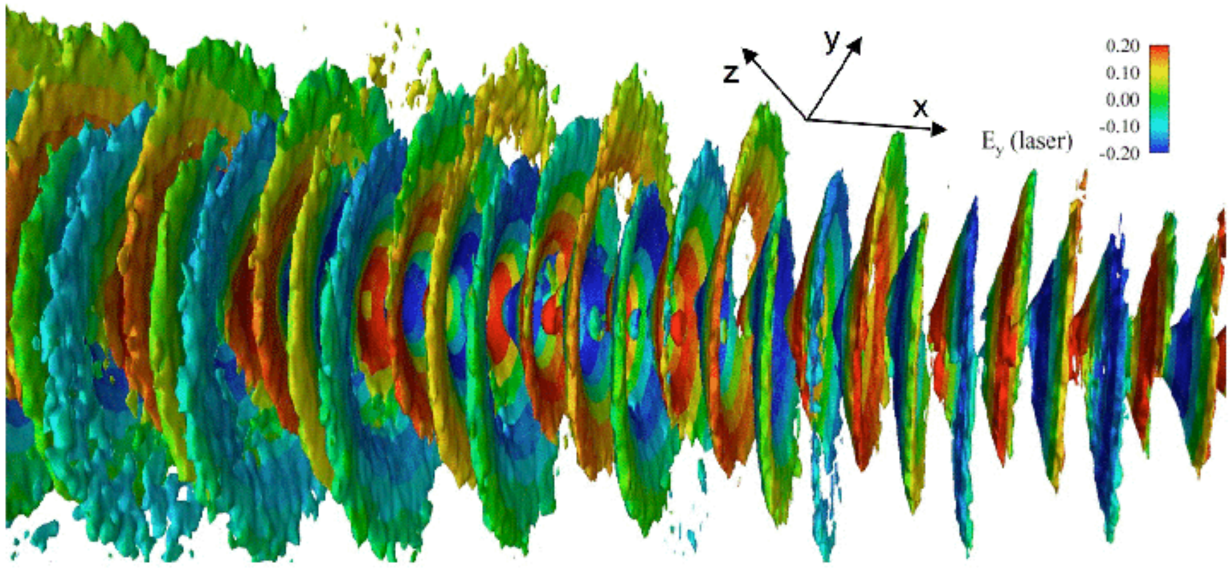


"Minimizing laser-plasma instabilities in the NIF hohlraum is a key to achieving ignition."
- LLNL web site

Inertial Confinement Fusion

LPI (Laser Plasma Interaction) an issue

- **Laser scattering:** Too little compression
- **Laser scattering:** Asymmetric compression
- **e$^-$ Preheating:** Harder to compress hot plasma



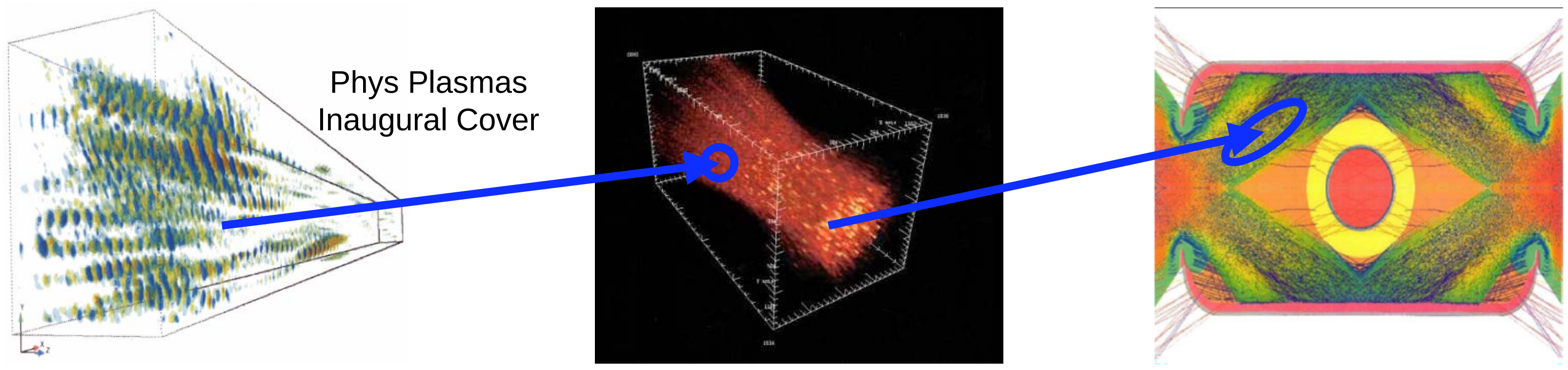
LPI Nonlinear Saturation (Yin *et al*, Phys Rev Lett, 2007)

The Petascale Challenge

In 2010, ICF ignition experiments start
at Livermore's National Ignition Facility (NIF)

The multi-billion dollar question:
What is the risk from LPI?

Petascale computing can address this issue



LANL VPIC
LPI modeling

LLNL pF3D
laser modeling

LLNL Hydra
ICF modeling

Computational Science in Action

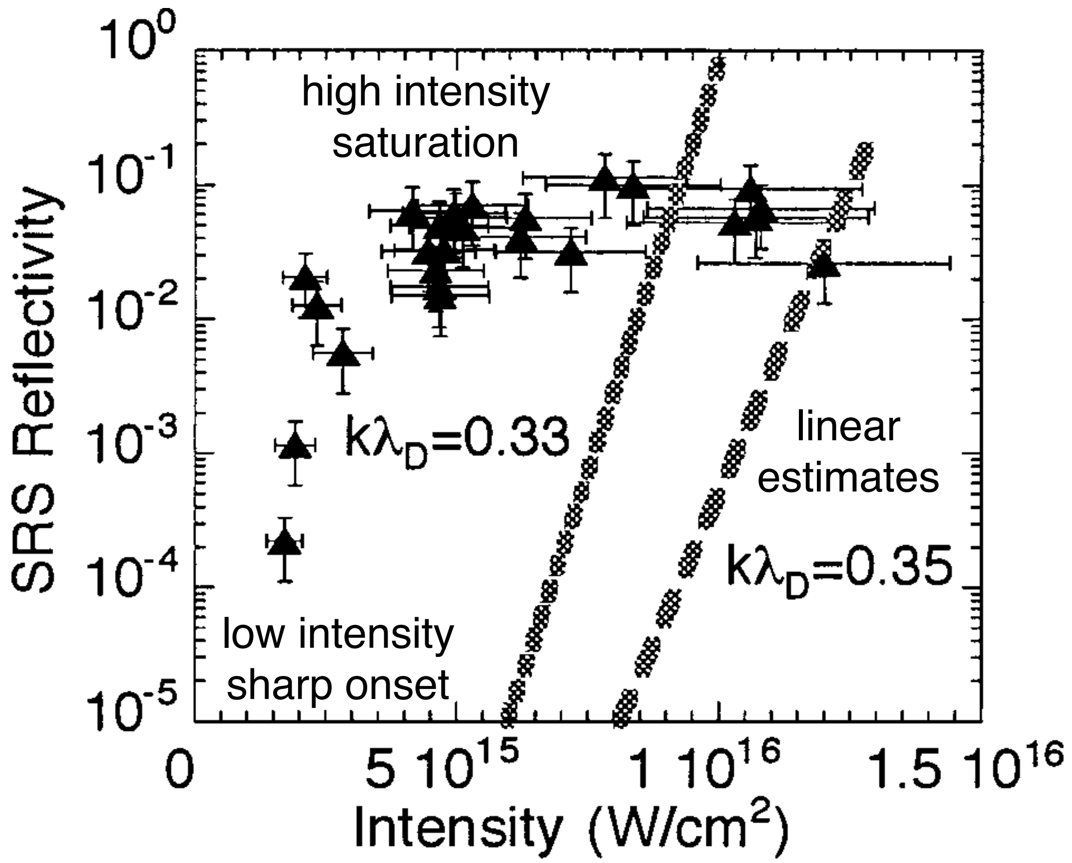
Linear theory for SRS (Stimulated Raman Scattering) in LPI developed

Drake *et al*, Phys Fluids, 1974

Trident experiments observe unexplained behavior

Montgomery *et al*, Phys Plasmas, 2002

Trident Experiments (527 nm, f/4.5 Gaussian beam, T_e=700eV)



Computational Science in Action

VPIC identifies key physics

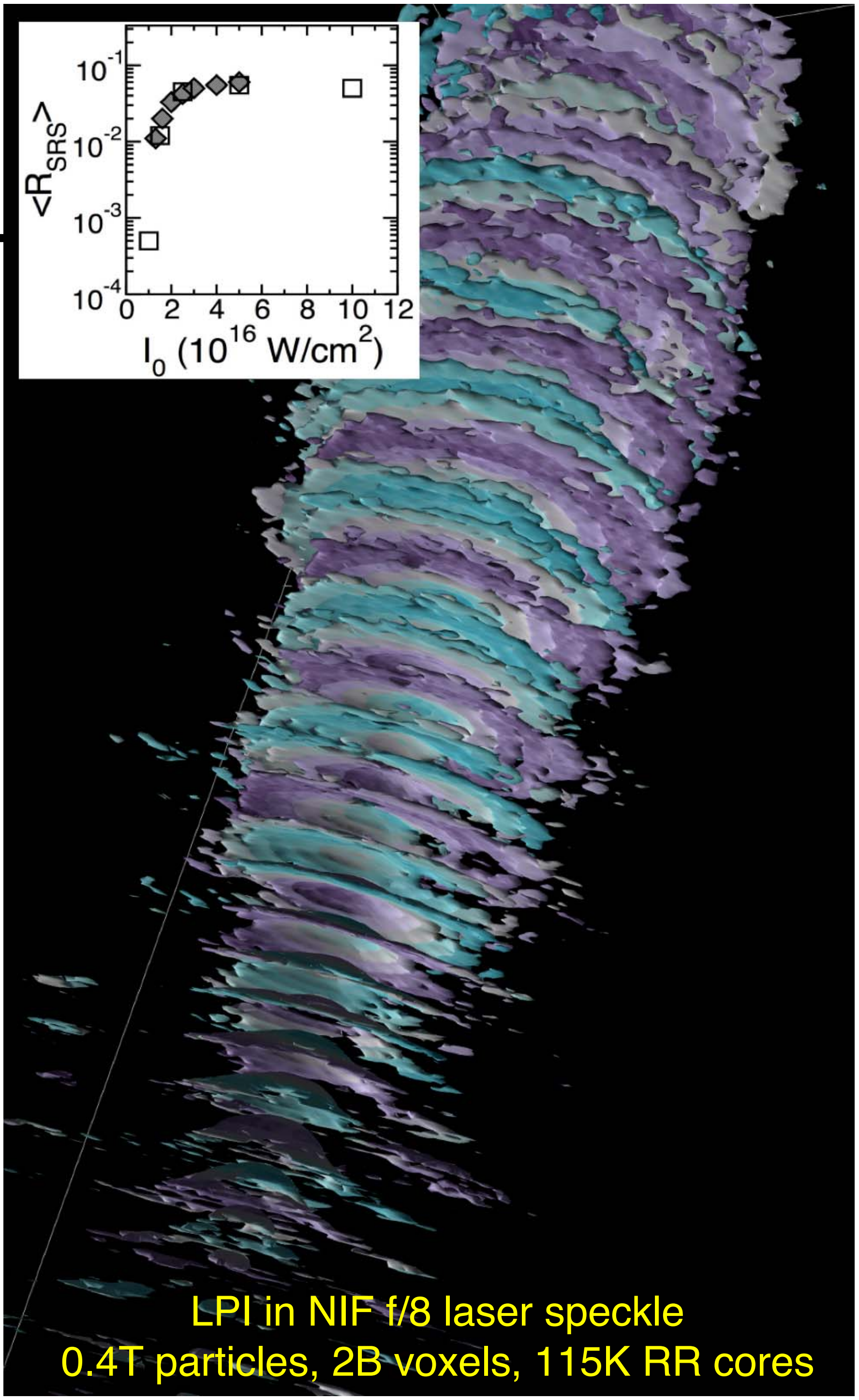
Plasma wave bowing, self-focusing, filamentation and trapped particle modulational instability cause rapid onset and saturation (Yin *et al*, Phys Rev Lett, 2007)

Reflectivity agrees with experiment

Simulation insights lead to non-linear SRS theories

Rose and Yin, Phys Plasmas, 2008, Yin *et al*, Phys Plasmas, 2009

VPIC now being used on Roadrunner to understand and predict LPI in NIF



LPI in NIF f/8 laser speckle
0.4T particles, 2B voxels, 115K RR cores

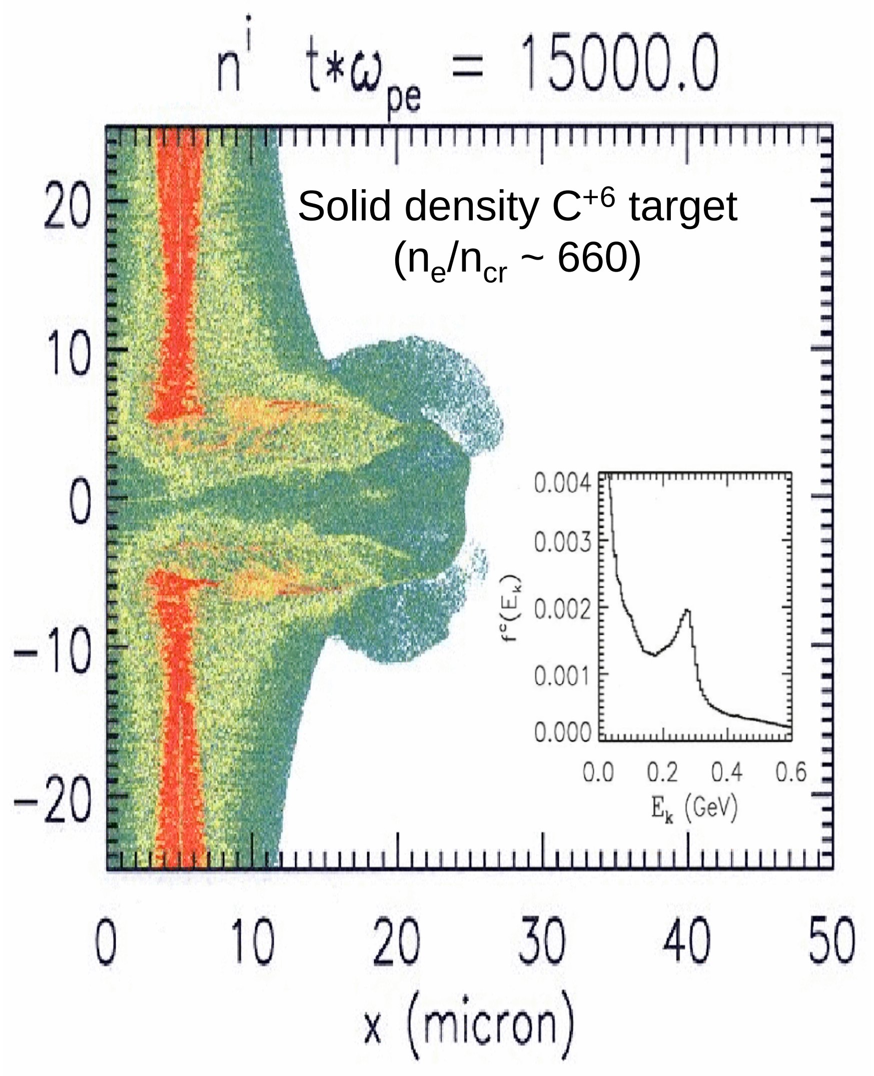
Laser Ion Acceleration

High energy C^{+6} beams observed from an ultra-intense short laser pulse incident on a thin foil

Via target normal sheath acceleration process (Hegelich *et al*, Nature, 2006, Albright *et al*, Phys Rev Lett, 2006)

VPIC corroborates and discovers a process for higher energies

Relativistic effects make foil transparent for ultra-high contrast pulses and thinner foils, allowing pulse to “breakout” and accelerate ions (Yin *et al*, Laser and Particle Beams, 2006)



Laser Ion Acceleration

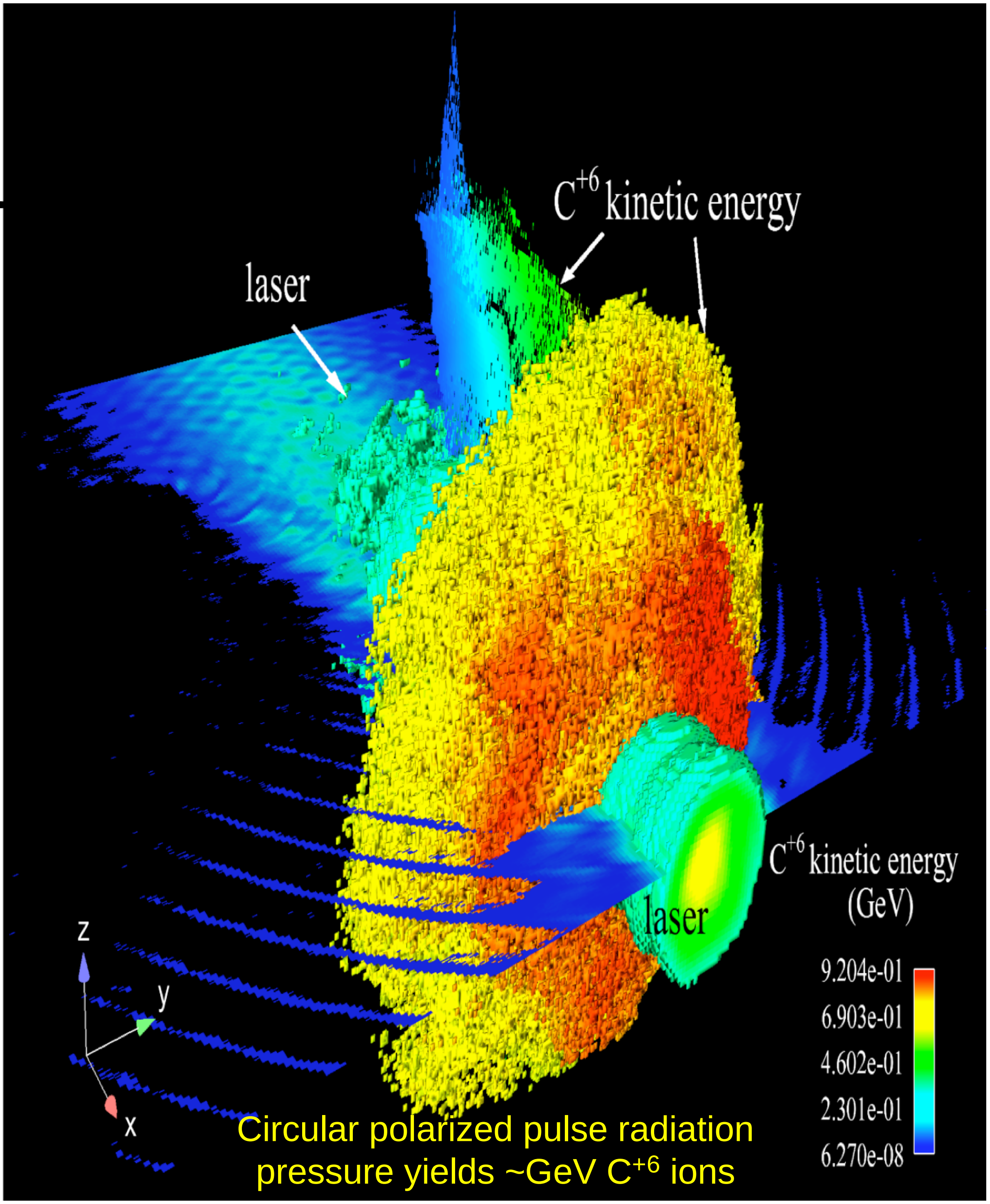
Simulation insights lead to new acceleration theories

Relativistic Buneman instability for linear polarization (Albright *et al*, Phys Plasmas 2007)

VPIC prediction experimentally confirmed

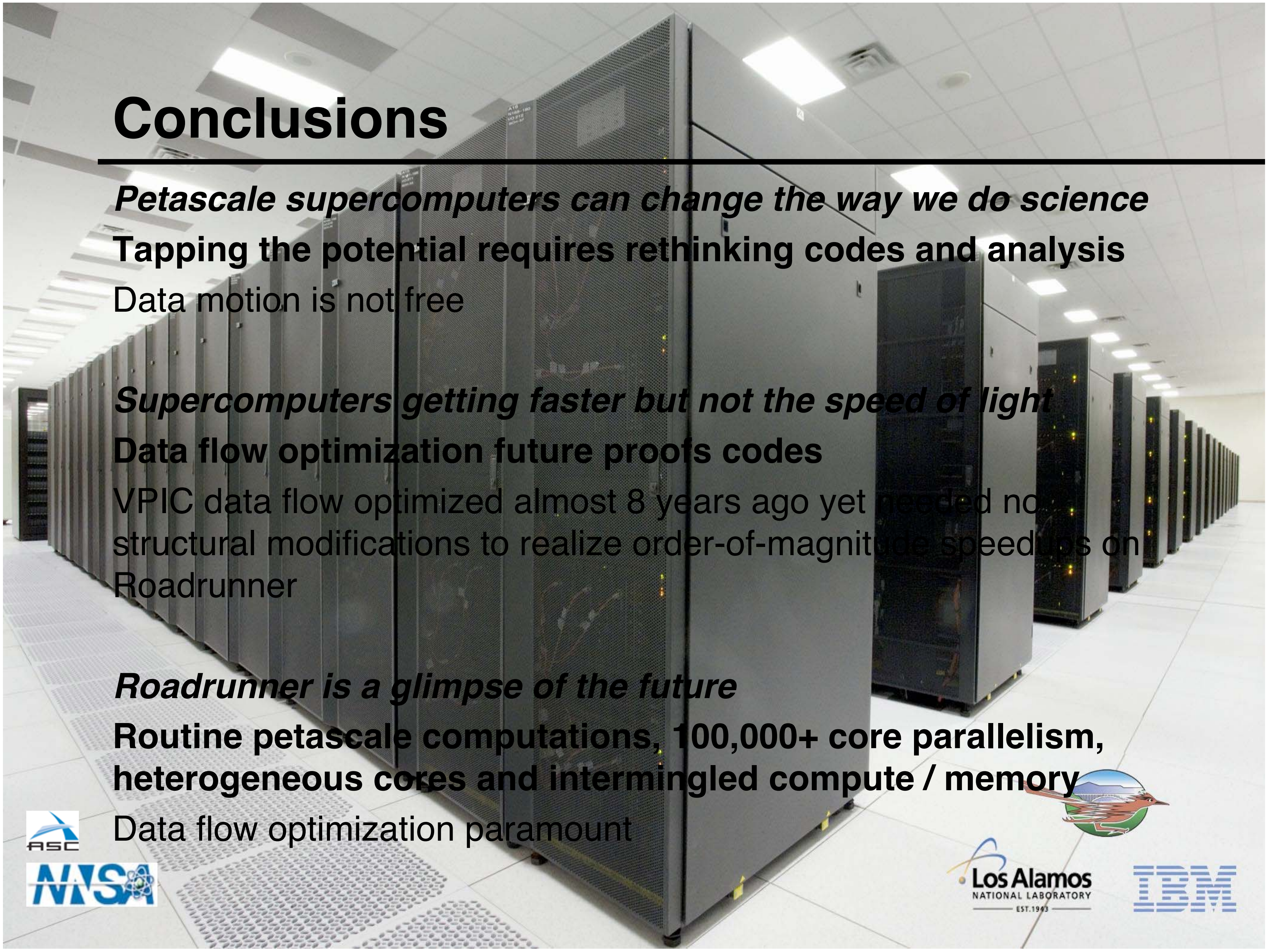
Prediction drove Trident's redesign

Henig *et al*, Phys Rev Lett, 2009 (in press)



Circular polarized pulse radiation pressure yields ~GeV C^{+6} ions

Los Alamos



Conclusions

Petascale supercomputers can change the way we do science

Tapping the potential requires rethinking codes and analysis

Data motion is not free

Supercomputers getting faster but not the speed of light

Data flow optimization future proofs codes

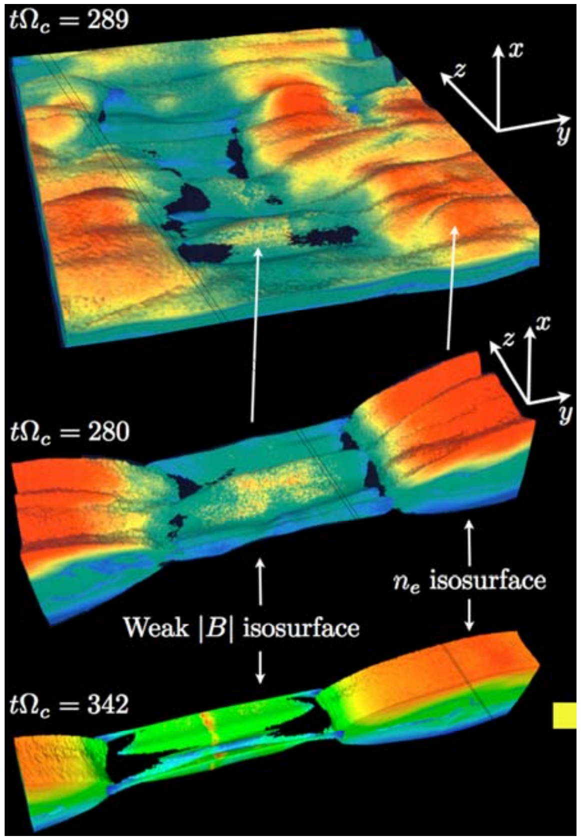
VPIC data flow optimized almost 8 years ago yet needed no structural modifications to realize order-of-magnitude speedups on Roadrunner

Roadrunner is a glimpse of the future

Routine petascale computations, 100,000+ core parallelism, heterogeneous cores and intermingled compute / memory

Data flow optimization paramount

Acknowledgments



Harris sheet tearing (Yin *et al*, Phys Rev Lett, 2008)

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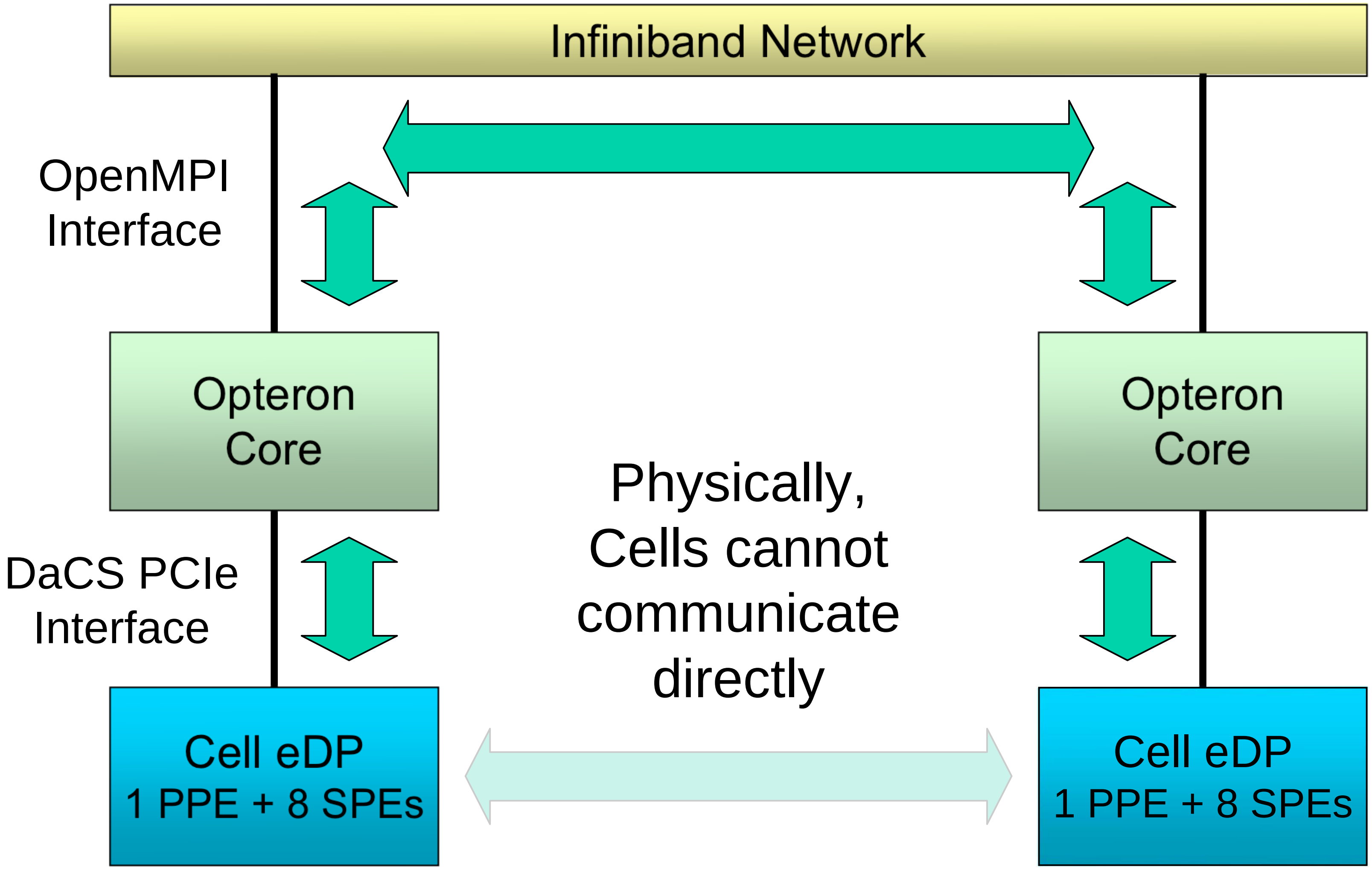
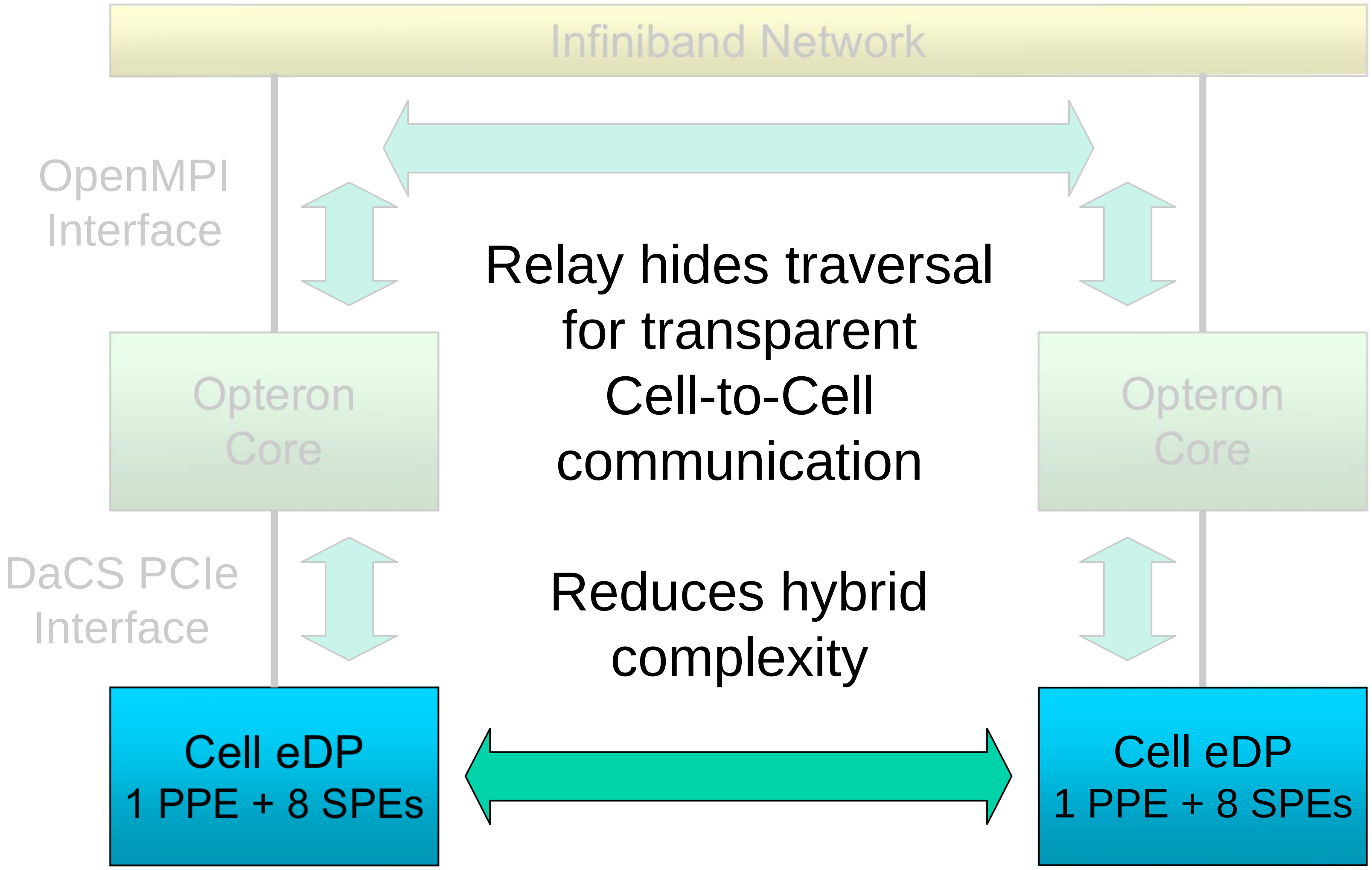
Los Alamos

Relay Library



Relay Library



Relay hides traversal for transparent Cell-to-Cell communication

Reduces hybrid complexity